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Model (ROM2.0): Evaluation on 1980 NEROS Data Bases

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EPA REGIONAL OXIDANT MODEL (ROM2.0): EVALUATION ON 1980 NEROS DATA BASES

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ABSTRACT

The second generation U.S. EPA Regional Oxidant Model (ROM2.0) has been evaluated for the northeastern United States using the 1980 NEROS data bases. The theoretical basis of the model and its structure and organization are described. The data bases available from the summer 1980 period include the routine monitoring data of meteorological and air quality parameters from the National Weather Service and the SAROAD network. In addition, several extensive field measurement projects were sponsored during the summer of 1980 in the northeastern U.S. on regional and urban scales. Supplementary meteorological and air quality measurements were made at the surface as part of these field projects. In addition, an extensive measurement campaign was conducted aloft using several aircraft also on regional and urban scales. Also, a complete emissions inventory was assembled for the 1980 base year for use in air quality modeling. The emissions inventory was composed of anthropogenic and biogenic components.

The ROM2.0 evaluation was conducted using quasi-deterministic and diagnostic techniques. Strict temporal and spatial pairing between observations and predictions was not used in the analysis. Model simulation was conducted during the period of July 12 to August 31, 1980. The simulation was begun under relatively clean tropospheric conditions to circumvent the difficult problem of initialization. Model performance over the simulation period showed an overall 2% overprediction of the daily surface maximum O_3 concentrations. ROM-predicted concentrations, however, had a narrower range for ambient O_3 with underestimation of highest values and overestimation of lowest values. The ROM underpredicted daily maximum O_3 values at the 75th percentile for group 1 sites by 30–50 ppb during major episodes. Ratios of observed to predicted NO_x and NMHC concentrations during the 06–09 h, LDT period were 2.5 and ≈ 5 , respectively, for surface observations. The spatial extent and concentrations of urban O_3 plumes were generally simulated well, although a bias in the transport direction along the East Coast caused frequent misalignment of the plumes. Model performance analyses using aircraft data showed the model to underpredict the regional O_3 tropospheric burden under episodic conditions, although individual plumes were modeled well.

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1 INTRODUCTION

The initial development of a regional (≈ 1000 km) air quality simulation model began in the late 1970's after the realization that photochemical smog often extended beyond individual urban areas to entire sections of the U.S. Interstate transport of O_3 and its precursors was observed during field programs of the 1970's, especially in the Northeastern U.S. (Wolff and Lioy, 1980). Long-range transport of O_3 and precursors and multi-day chemical effects could not be properly treated by existing urban-scale photochemical models. The need became apparent for an appropriate simulation model to test the effectiveness of particular emissions control strategies on O_3 concentrations in urban airsheds as well as region-wide.

The first generation EPA Regional Oxidant Model (ROM1.0) became operational in 1984 (Lamb, 1983, 1984; Lamb and Laniak, 1985). It was a test bed for the future production version of the model, the second generation ROM2.0. The earlier model contained a very condensed chemical kinetic mechanism, could not treat natural hydrocarbons, had limited treatment of vertical mass flux induced by clouds, had constant layer depths, and contained very limited terrain effects. Nevertheless, ROM1.0 was used for extensive testing of various emission control scenarios in the Northeast U.S. A limited evaluation of the model was performed using ambient air quality data (Schere, 1986). The network design of the ROM data preprocessor system including the complex data communication channels within the system was performed during the testing of the the first generation model. Various methods for chemical and physical process simulation were tested within the ROM1.0 system as well.

A large field project in the Northeast U.S. was planned and conducted concurrently with the ROM model development effort. The purposes of the field program were to gather data to better understand the important processes responsible for photochemical smog on the regional scale so they could be properly simulated by the model and to provide a data base for testing and evaluation of the model. The field program was carried out over two summer periods during 1979 and 1980. Measure-

ments were taken from Ohio and Michigan to the East Coast, both in regional and in local projects. Extensive aircraft measurements supplemented the ground-based network. The data base from 1979 was used primarily in the model development, testing, and evaluation phases of ROM1.0. The 1980 data base was used almost exclusively for model evaluation of ROM2.0.

ROM2.0 became operational in 1987. This second generation version of the model was to become the production version. It included a more sophisticated, contemporary chemical kinetic mechanism capable of treating both anthropogenic and natural precursor species. The ROM2.0 system also corrected most of the deficiencies and simplifications of the first generation system, such as cloud-induced mass flux, variable layer depths, and terrain effects. Once operational, ROM2.0 was used for extensive testing of emissions control scenarios within the Northeast U.S. for EPA's Office of Air Quality Planning and Standards (OAQPS), as well as the Vice President's Commission on Clean Coal Technology, and the Congressional Office of Technology Assessment.

This document presents the results of the evaluation of ROM2.0 on the 1980 Northeast U.S. data base. Emphasis is placed on the comparison between predicted and observed O_3 concentrations, although NO_x and hydrocarbons are evaluated also, to the extent that the data allow. Ground-based and aircraft data are used in the analysis. Statistical, graphical, and spatial analyses are presented.

The purpose of this evaluation is essentially a *confidence building* exercise in the ROM2.0 for its use as an air quality planning tool. Model evaluation against ambient data is a necessary, but not sufficient, condition for evaluating an air quality model for use in the regulatory arena of agencies such as the U.S. EPA, and State and local air pollution boards. Model evaluation is not a singular event; it is an on-going process. The evaluation reported here is the first, but certainly not the last, for the second generation ROM. It is significant not only because it is the first major evaluation, but also for the enhanced ambient data base that is used. Subsequent evaluations will add to the knowledge of how the ROM performs under different meteorological, geographical, and air quality conditions and, thereby increase the understanding and confidence in its use.

2 THE REGIONAL OXIDANT MODEL

2.1 MODEL OVERVIEW

2.1.1 Theoretical Basis

The ROM has been designed to simulate most of the important chemical and physical processes responsible for the production of photochemically produced O_3 on scales of 1000 km, or several days of transport time. These processes include horizontal transport, atmospheric chemistry, nighttime wind shear and turbulence episodes associated with the nocturnal jet, cumulus cloud effects on vertical mass transport and photochemical reaction rates, mesoscale vertical motions induced by terrain and the large scale flow, terrain effects on advection, diffusion, and deposition, sub-grid scale chemistry processes, emissions of natural and anthropogenic precursors, and deposition. They are mathematically simulated in the 3-D Eulerian model with $3\frac{1}{2}$ vertical layers including the boundary layer and the capping inversion or cloud layer. Horizontal resolution is $\frac{1}{4}^\circ$ of longitude by $\frac{1}{6}^\circ$ of latitude, or about 18.5 km.

Lamb (1983, 1984) presents detailed descriptions of the theoretical basis and design of the ROM. This section presents a brief overview of the model including some of its unique features. Figure 2.1 displays the vertical structure during daytime conditions. The top three layers are prognostic (predictive) and are free to locally expand and contract in response to changes in the physical processes occurring therein. During an entire simulation period horizontal advection and diffusion and gas phase chemistry are modeled prognostically in the upper three layers. The bottom layer is a shallow diagnostic surface layer designed to approximate the sub-grid scale effects on chemical reaction rates from a spatially heterogeneous emissions distribution. The design and implementation of this surface layer, layer 0, has not been fully accomplished yet. Therefore, ROM predictions from layer 1 are used as surrogates for surface concentrations.

Layers 1 and 2 model the depth of the well-mixed layer during the day. In local areas where strong winds exist and the surface heat flux is weak there can exist substantial wind shear in the lowest few hundred meters above ground. This phenomenon can be treated separately in layer 1. Also, over large lakes or near seacoasts there often exists a thermal internal boundary layer that is modeled in layer 1. Deposition on terrain features that protrude above the surface layer are also handled here. At night, layer 2 represents the remains of the daytime mixed layer. As stable layers form near the ground and suppress turbulent vertical mixing a nocturnal jet forms above the stable layer and can transport aged pollutant products and reactants considerable distances. At night, emissions from tall stacks and warm cities are injected directly into layers 1 and 2 aloft. Surface emissions are specified as a mass flux through the bottom of layer 1.

During the day, the top model layer, layer 3, represents the synoptic scale subsidence inversion, the base of which is typically 1-2 km above the ground. Relatively clean tropospheric air is assumed to exist above layer 3 at all times. If cumulus clouds are present, an upward flux of O_3 and precursor species is injected into the layer by penetrative convection. At night, O_3 and the remnants of other photochemical reaction products may remain in this layer and be transported long distances downwind. These processes are included in layer 3.

When cumulus clouds are present in a layer 3 cell the upward vertical mass flux from the surface is partially diverted from injection into layer 1 to injection directly into the cumulus cloud of layer 3. In the atmosphere, strong thermal vertical updrafts, primarily originating near the surface in the lowest portion of the mixed layer, feed young growing cumulus clouds with vertical air currents that extend from the ground to well above the top of the mixed layer in one steady upward motion. The dynamic effects of this transport process and daytime cloud evolution may have significant effects on the chemical fate of pollutants caught up in the process. For example, fresh emissions from the surface layer may be injected into a warm thermal and rise, essentially unperturbed, to the top of the mixing layer where they enter the base of a growing cumulus cloud. Within the cloud the chemical processes of ambient pollutant species are suddenly altered by the presence of liquid water and the attendant attenuation of sunlight. The presence of young cumulus clouds implies that the atmosphere above the earth's boundary layer is too stably stratified for thermals to penetrate higher. When this happens the air composing the tops of these clouds dives back into the mixed layer and is heated by compression on its descent. Ultimately, the parcel arrives again at the surface level where new emissions may be injected into it and ground deposition may occur, and the process may begin again. The time required for one complete cycle would typically be 30-50 minutes with perhaps $\frac{1}{10}$ of the time spent in the cloud stage.

Within the ROM system, a sophisticated sub-model simulates this cloud flux process and its impact on the material fluxes among all the model's layers. In

the current implementation of the chemical kinetics, liquid phase chemistry is not modeled and thus part of the effects from the cloud flux processes are not accounted for in the simulations. Future versions of the chemical kinetics may include liquid phase reactions. The magnitude of the mass flux proceeding directly from the surface layer to the cloud layer is modeled as being proportional to the observed amount of cumulus cloud coverage and inversely proportional to the observed depth of the clouds.

Horizontal transport within the ROM system is governed by hourly wind fields interpolated from periodic wind observations made from upper air soundings and surface measurements. During the nighttime simulation period the lowest few hundred meters of the atmosphere above the ground may become stable as a radiation inversion forms near the ground. This entire layer is "decoupled" from the rest of the old daytime mixed layer. Wind speeds increase in this inversion layer and the nocturnal jet forms, capable of carrying O_3 , other reaction products, and emissions injected aloft considerable distances downwind. This phenomenon is potentially quite significant in modeling regional scale air quality and is treated in ROM layer 1. Because standard weather observations of winds do not have the spatial or temporal resolution necessary to diagnostically determine this flow over large distances with any confidence, a sub-model within the ROM system was developed to simulate the nighttime flow regime in layer 1 only.

The prognostic flow sub-model is activated only when a surface inversion is present over most of the model domain. At all other times the flow in layer 1 is determined from interpolation of observed winds. The nighttime flow regime within layer 1 is influenced by buoyancy, terrain, warm cities, geostrophic forcing, and frictional forces. These are all accounted for in the flow model formulation. Solution of the wind sub-model equations produces estimates of the wind components as well as the depth of the inversion layer for all grid cells in layer 1.

The chemical kinetic mechanism embedded in ROM2.0 is the Carbon Bond 4.0 (CB-4) set of reactions (Whitten and Gery, 1986). This mechanism simulates the significant reaction pathways responsible for gas-phase production and destruction of photochemical smog constituents on regional scales. The mechanism consists of 70 reactions including 28 individual species. The ROM's chemical solution scheme makes no *a priori* assumptions concerning local steady-states. Therefore, all species are advected, diffused, and chemically reacted within the model domain.

CB-4 contains a standard set of reactions for atmospheric inorganic chemistry, including O_3 , NO, NO_2 , CO, and other intermediate and radical species. Its organic chemistry is partitioned along reactivity lines based on the carbon-structures of the organic molecules. Nine individual categories of organics are represented, which attempt to account for the chemistry of the hundreds of organic molecules existing in the ambient atmosphere. They include ETH, an explicit representation of ethylene;

FORM, an explicit representation of formaldehyde; OLE, a double-bonded lumped structure including two carbons; PAR, a single bond, single carbon structure¹; ALD2, the oxygenated two-carbon structure of the higher aldehydes²; TOL, the aromatic structure of molecules with only one functional group; XYL, the structure of molecules with multifunctional aromatic rings; ISOP, a four-carbon surrogate for the biogenic isoprene molecule³; and NONR, a single carbon organic structure not significantly participating in the reaction sequence.

Two classes of biogenic hydrocarbon are included in a separate natural area source emissions inventory used by the ROM. One, isoprene, a molecule principally emitted by deciduous trees, is treated by the ISOP species in CB-4. The other, monoterpenes, a class of natural hydrocarbons emitted principally by coniferous trees, is not treated explicitly in CB-4. The surrogate monoterpene molecule, α -pinene, which consists of 10 carbons, is apportioned to the existing CB-4 categories as 1 OLE and 8 PAR.

2.1.2 Structure and Organization

The key components of the ROM2.0 modeling system are illustrated in Figure 2.2. The system requires six types of "raw" data inputs: air quality, meteorology, emissions, cloud cover, land use, and topography. These raw data are manipulated by a hierarchical network of preprocessors which range in function from simple reformatting of emissions data to generating the complex families of wind fields which drive the atmospheric transport. These processors are interconnected by their requirements for and production of data. The ultimate product of the processor network is a collection of data files which can be categorized into two types: processor input files (PIF) and model input files (MIF). PIFs contain partially processed data required as input to higher level processors. MIFs also provide input to a number of higher level processors; however, they primarily contain the parameter fields which are transformed into matrix elements and variables required by the model algorithms.

The processors are organized into six distinct hierarchical levels. Level 1 processors interface directly with the "raw" input data sets. These "raw" data sets have, in fact, undergone extensive quality control. Subsequent levels transform the raw data into the gridded fields of temporally and spatially varying parameter values needed by the highest levels of the processing network. Processors at any level can interface directly with the B-Matrix compiler (BMC), described below,

¹Note that the single-bonded constituents of other types of molecules, such as olefins and aromatics, are also treated as one-carbon PAR species.

²Note that internal olefins are treated by assuming that they have already reacted in the atmosphere to form two higher aldehydes (2 ALD2).

³The remaining carbon of the isoprene molecule is treated as 1 PAR.

by production of model input files. This multi-level organization is important to the network because it clearly delineates the sequence of program execution. Processors at the same level may execute simultaneously. However, a processor at any given level must wait until all preceeding processors from lower levels along its input data paths have been completed. Formal definition of all data/processor relationships and automation of processor executions are essential to ensure consistency and validity of MIFs.

The program which serves as the interface between the model input files and the algorithms describing the governing processes is called the B-Matrix Compiler (BMC) because it functions similarly to a computer language compiler which transforms high level language commands into machine/algorithm specific representation. The BMC mathematically combines physical parameters such as wind components, horizontal eddy diffusivities, etc. into the complex coefficients required for solution of the governing equations. These coefficients can no longer be equated with physical reality; they are purely mathematical entities related specifically to the form of the generalized finite difference algorithms used by the ROM.

The core of the ROM system is a set of algorithms which solves the coupled set of generalized finite difference equations that describes the governing processes in each layer of the model. These governing equations have been expressed in a form which allows the chemical kinetics, advection, and vertical flux to be treated independently. The chemistry module exchanges information with algorithms of the governing equations via two vectors. One vector contains the net production rate of each species and the other vector contains the net destruction rate. Such design simplifications enhance the flexibility of the model and have been extended to allow interchange not only of the chemistry mechanism, but of all theoretical formulations of the physical and meteorological processes, i.e., the processors.

Thus the structure of the ROM system provides a flexible modeling framework with both permanent and interchangeable components. The permanent components are:

- the algorithmic form of the governing equations
- the B-Matrix Compiler
- the processor and model input files
- the data interfaces between components and processors.

The interchangeable components consist of the algorithms used to simulate the physical and chemical processes of the ROM system. Thus, for example, the chemical kinetic mechanism is an interchangeable component.

The formal design specification for the ROM system intentionally separates functional (interchangeable) components from "fixed" data interfaces which are part of the permanent component set. Once this general modeling framework is operational, continuous upgrading to state-of-the art methodologies is not only feasible, but also practical. The long term usefulness of this framework for atmospheric modeling research and applications tremendously outweighs any additional efforts required to develop flexibility in the framework rather than redevelop a new model. Ultimately, the difference in effort is primarily in the design, and not in the implementation.

2.2 SUMMARY OF ROM APPLICATIONS

Since ROM1.0 became operational in 1984 there have been numerous applications with the first and second generation models performed to date (Lamb, 1985, 1986, 1987, 1988; Schere, 1986; Pierce and Schere, 1988; Possiel *et al.*, 1988). Most of these applications have been in support of regulatory analyses to study the effects of various proposed emission control strategies on O₃ concentrations. Several of the applications have been of a more basic research nature, such as simulations to support model evaluation with ambient data or to test the sensitivity of the model's O₃ predictions to the biogenic hydrocarbon emissions. As of yet there has been no systematic sensitivity set of simulations performed, although this is planned for the future.

All model simulations have been performed for one or both of two existing domains: the Northeast U.S. (NE) domain, and the Southeast U.S. (SE) domain. They are shown in Figures 2.3 and 2.4, respectively. Both domains are the same size, 60 cells in the east-west direction, and 42 cells in the north-south direction, giving a total domain size of approximately 1100 km by 780 km.

Base case simulations have been performed for periods during the summers of 1979 and 1980 with ROM1.0 for the NE domain, and for periods during the spring and summer of 1980 with ROM2.0 for the NE and SE domains. While the same base case meteorological and air quality data bases have been used for all simulations within the same year, the emissions inventories have varied. The 1979 simulations used the 1979 source emissions inventory assembled as part of the Northeast Corridor Regional Modeling Project (NECRMP) sponsored by the EPA (Sellars *et al.*, 1982). The 1980 simulations with ROM1.0 used the version 4.2 inventory for 1980 developed for the National Acid Precipitation Assessment Program (NAPAP) (Toothman *et al.*, 1984) and the 1980 simulations with ROM2.0 used the NAPAP5.3 inventory (Wagner *et al.*, 1986). Methodology differences between the various inventories have led to significant differences in emission values.

The base case and control strategy simulations have been performed for various episodic periods, typically lasting 10–15 days. Analyses for welfare effects from O_3 , such as on crops and forests, require seasonal information as well as episodic concentration data. A technique was developed by Lamb (1988) to extrapolate the simulation results to a full O_3 season, based on the ROM results for several selected episodes from within that season. ROM2.0 results have been seasonally extrapolated for many of the 1980 simulations performed.

Table 2.1 presents a summary of the specific simulations performed with the ROM model to date. The individual emissions control strategies indicated in the table are defined below.

VOC0 Base emissions projected to 1987 including the effects of existing controls. Largest changes in VOC emissions; some smaller changes to NO_x emissions.

VOC1 Base emissions from 1980 reduced to include the effects of existing VOC controls in 1982 State Implementation Plans. Only VOC emissions are affected.

VOC2 VOC1 plus additional reductions expected by 1995 due to the Federal Motor Vehicle Control Program (FMVCP).

VOC3 VOC2 plus additional reductions in the Northeast Corridor, Pittsburgh, Cleveland, and Detroit.

VOC4 VOC3 including a higher level of reductions, up to 90% control in the Northeast Corridor.

NO_x 1 NO_x controls on utility boiler emissions from 1980 resulting in a 39% cut in utility emissions (11% cut in regionwide NO_x).

NO_x 2 Utility/industrial boiler plus FMVCP NO_x controls only in Detroit (27% resulting cut in NO_x emissions) and the Northeast Corridor (22% resulting cut). Overall 10% cut in regionwide NO_x .

NO_x 3 Utility/industrial boiler plus FMVCP NO_x controls applied regionally. (This resulted in a 22% cut in NO_x emissions for the Northeast Corridor, and a 27% cut in regionwide NO_x for the Northeast U.S. domain.)

NO_x 4 NO_x 3 except for $\approx 70\%$ cut in point source NO_x emissions in the Northeast Corridor.

In general, the results provided by the ROM2.0 control strategy simulations have shown that controlling VOC emissions alone reduces peak O_3 concentrations in urban areas and downwind. Controlling NO_x alone can have mixed effects on O_3

concentrations. Up to 20% increases in maximum O_3 concentrations were seen close-in to some urban areas, while there were localized decreases in rural area maximum O_3 concentrations, from 5 to 10% (Possiel *et al.*, 1988). Preliminary results from ROM simulations employing combined VOC and NO_x emissions controls show these controls to be more effective than VOC controls alone in some remote rural areas, although the effects can vary with meteorological conditions.

TABLE 2.1. SUMMARY OF ROM SIMULATIONS

Simulation Dates	Base Case or Control Strategy	Model	Purpose [†]	Seasonal Extrapolation [†]
Northeast U.S. Domain:				
Aug. 3-4, 1979	Base Case VOC0	ROM1.0	R, E	
		ROM1.0	R	
April 14-29, 1980	Base Case VOC1 VOC2 VOC3+NOx3	ROM2.0	R	✓
		ROM2.0	R	✓
		ROM2.0	R	✓
		ROM2.0	R	✓
July 12-17, 1980	Without biogenic HC emissions	ROM2.0	S	
July 12-26, 1980	Base Case	ROM2.0	R	✓
	VOC1	ROM2.0	R	✓
	VOC2	ROM2.0	R	✓
	NOx1	ROM2.0	R	
	NOx2	ROM2.0	R	
	VOC2+NOx3	ROM2.0	R	
	VOC3+NOx3	ROM2.0	R	✓
	VOC4+NOx3	ROM2.0	R	
	VOC4+NOx4	ROM2.0	R	
	With TSDF emissions	ROM2.0	R, S	
July 12-Aug. 31, 1980	Base Case	ROM2.0	E	
July 22-31, 1980	Base Case VOC0	ROM1.0	R	
		ROM1.0	R	
July 26-28, 1980	Base Case	ROM1.0	S	
	With other Δx , Δy grid sizes	ROM1.0	S	

TABLE 2.1. (continued)

Simulation Dates	Base Case or Control Strategy	Model	Purpose [†]	Seasonal Extrapolation [‡]
Aug. 22-31, 1980	Base Case	ROM2.0	R	✓
	VOC1	ROM2.0	R	✓
	VOC2	ROM2.0	R	✓
	NOx1	ROM2.0	R	
	NOx2	ROM2.0	R	
	VOC2+NOx3	ROM2.0	R	
	VOC3+NOx3	ROM2.0	R	✓
	With TSDF emissions	ROM2.0	R, S	
Southeast U.S. Domain:				
April 14-29, 1980	Base Case	ROM2.0	R	✓
	VOC1	ROM2.0	R	✓
	VOC2	ROM2.0	R	✓
	VOC2+NOx3	ROM2.0	R	✓
June 29-July 14, 1980	Base Case	ROM2.0	R	✓
	VOC1	ROM2.0	R	✓
	VOC2	ROM2.0	R	✓
	VOC2+NOx3	ROM2.0	R	✓
Aug. 18-Sept. 1, 1980	Base Case	ROM2.0	R	✓
	VOC1	ROM2.0	R	✓
	VOC2	ROM2.0	R	✓
	VOC2+NOx3	ROM2.0	R	✓
	With TSDF emissions	ROM2.0	R, S	
[†] E=Model evaluation study, S=Model sensitivity analysis, R=Regulatory analysis [‡] A ✓ indicates that this simulation was used, along with others, to extrapolate episodic model results to a full season.				

Layer Functions

Daytime

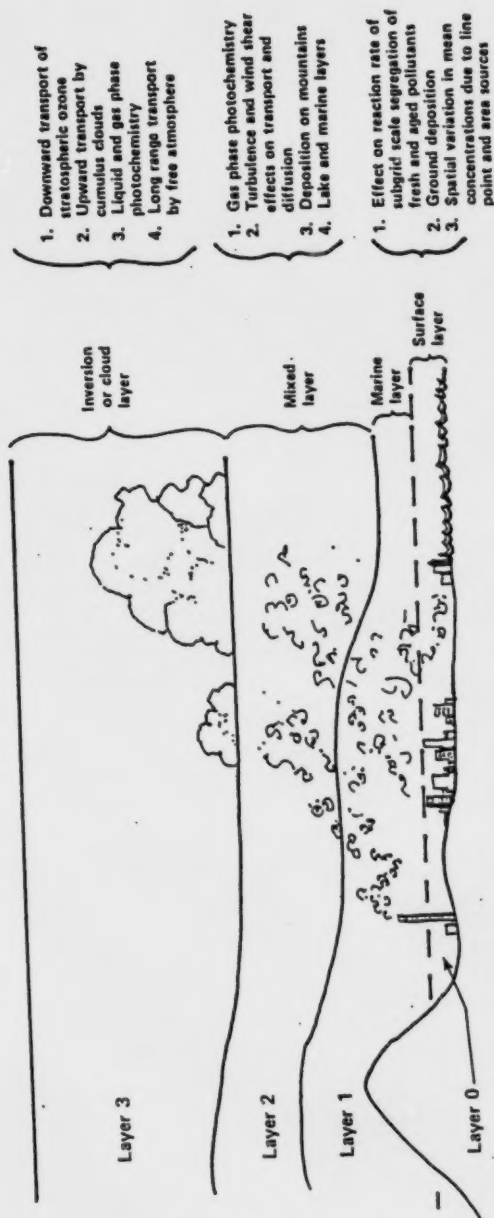


Figure 2.1. ROM vertical structure during daytime conditions.

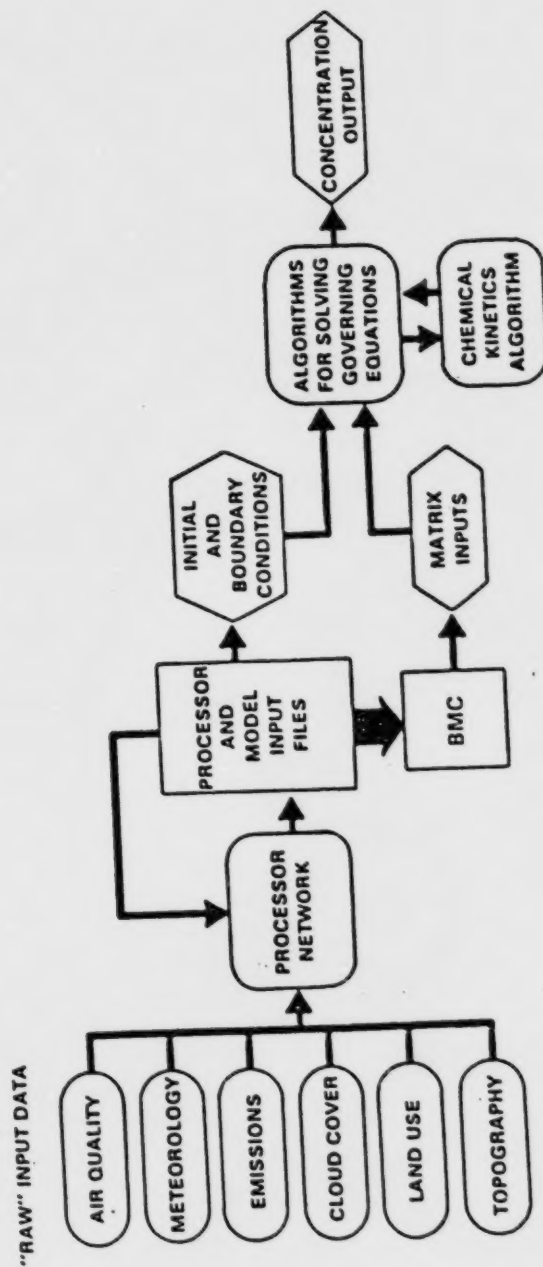


Figure 2.2. ROM system overview.

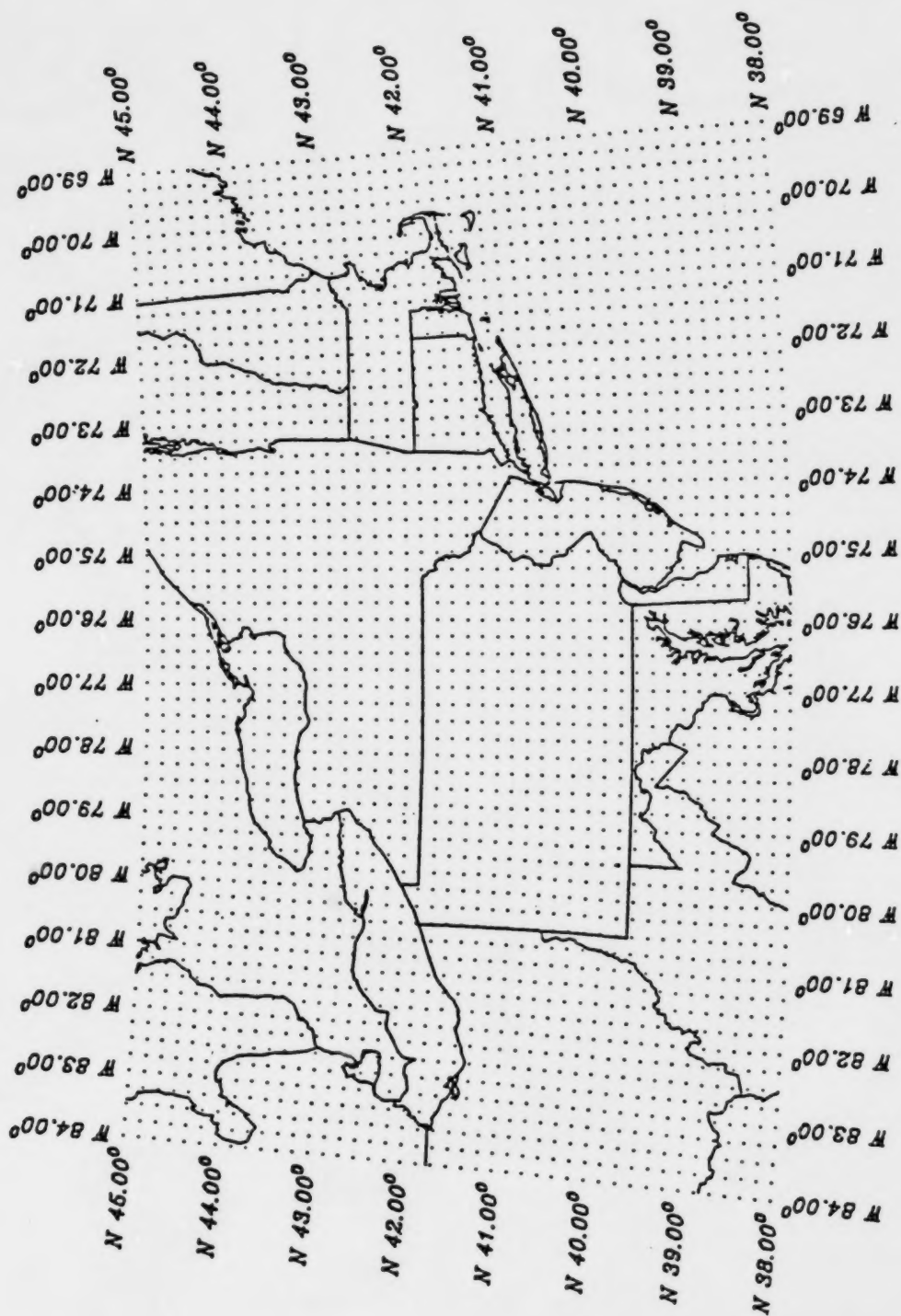


Figure 2.3. Northeast U.S. ROM domain. Each dot represents a corner of a grid cell.

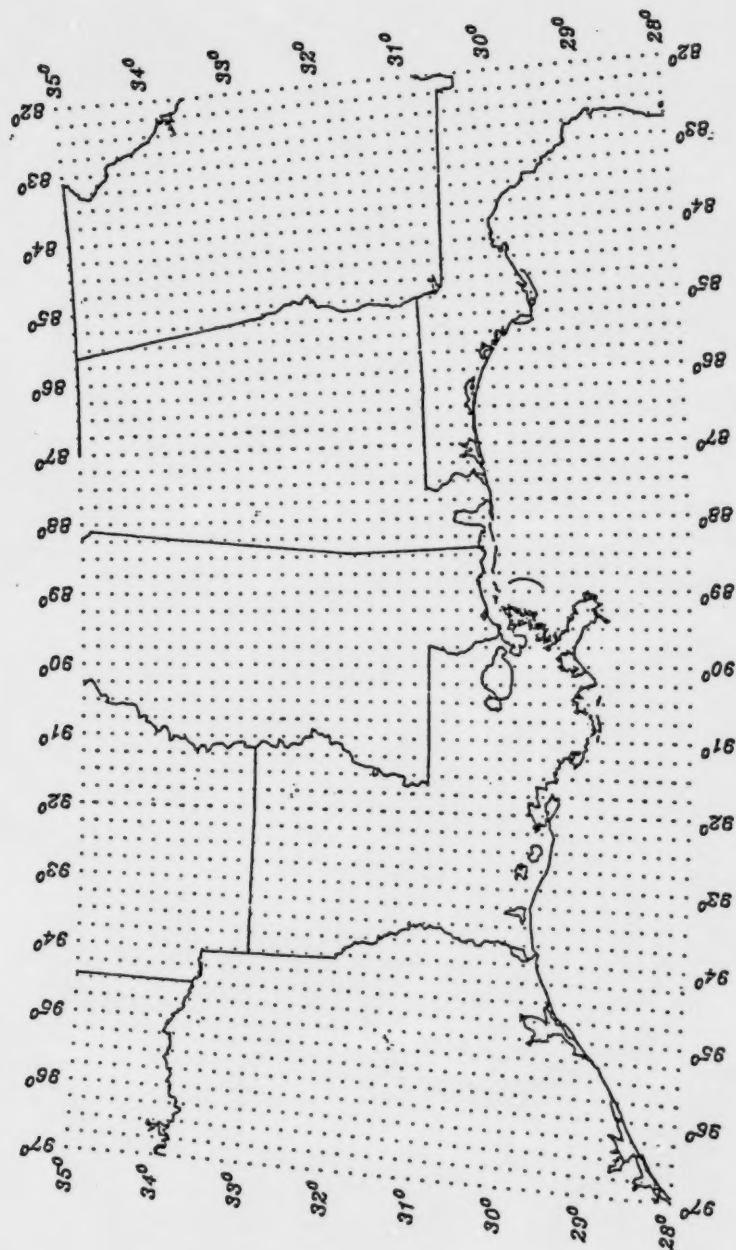


Figure 2.4. Southeast U.S. ROM domain. Each dot represents a corner of a grid cell.

3 MODEL APPLICATION

The particular application of ROM2.0 used in this evaluation exercise was conducted on a historical data base, with model simulation beginning at 1200 h, LST on July 12, 1980 and continuing through 1200 h, LST on August 31, 1980. The domain of application is that of the Northeast U.S., shown previously in Figure 2.3. The simulation was not reinitialized at any time after it began. It was continuous in time, performed in contiguous 3-day segments, with the simulation results from the final step of one segment used as restart conditions for the initial step of the next segment. This time period contained several significant O₃ episodes in the Northeastern U.S., with measured concentrations as high as 300 ppb. This section discusses the data bases used to provide the required data needed to perform the simulation and the data bases used for comparison of observed concentrations with simulation results. There is also a discussion of the use of air quality data in providing initial and boundary conditions for the model simulation.

3.1 DATA BASES

The data bases used in this project include meteorological, air quality, and emissions components. The ROM requires all three types of data for simulating regional air quality. The performance evaluation of the model predictions primarily requires the air quality data base. The summer 1980 period was chosen for this effort because it coincided with several major field projects, conducted in the Northeast U.S., designed to study the regional and urban O₃ problems. These projects provided special data bases which supplemented the standard air quality and meteorological measurements archived in EPA's SAROAD (Storage and Retrieval of Aerometric Data) system and collected by NOAA's National Weather Service (NWS), respectively. The model has been designed to run in an operational mode solely on these routinely collected data bases. The special study data bases are used for model evaluation and research on model parameterizations.

3.1.1 Standard Data Bases

The SAROAD data, supplemented by monitoring data in southern Ontario, Canada obtained from Environment Canada and the Ontario Ministry of the Environment, provided hourly measurements of O_3 , NO_2 , and NO_x at fixed monitoring sites within the model domain. The locations of these sites are indicated in the sections that follow. There were 214 sites where O_3 measurements were made, 107 sites for NO_2 , and 65 sites for NO_x during the summer 1980 period. Most of the monitoring sites are within or near urban areas.

Appendix A contains spatial maps of the daily maximum O_3 concentrations recorded at each of the monitoring sites in the SAROAD and southern Ontario networks for the simulation period. There is one map for each day of the period, and all sites do not appear on each map because of intermittent maintenance or calibration problems with the monitors.

Hourly surface meteorological measurements were available from ≈ 200 stations within the ROM domain in the NWS and Canadian meteorological networks. The ROM preprocessors assimilate raw meteorological data on atmospheric pressure, temperature, moisture, winds, and clouds from these locations. Transport, diffusion, and thermodynamic processes within the modeling system are affected by these meteorological measurements. In addition to the surface measurements, the North American upper air sounding network contains 24 stations within and near the boundaries of the ROM domain where twice daily upper air soundings provided measurements of pressure, temperature, moisture, and winds. Nine of these stations are located within the ROM domain boundaries, and the frequency of soundings was increased to four times per day at these stations during "intensive" NEROS field study periods.

Appendix B contains copies of the U.S. surface weather map for 0700 h, EST for each day of the simulation period. While these maps do not indicate exact conditions as used by the ROM (since the ROM assimilates vertically integrated data), they provide an indication of the overall meteorological conditions as they existed for any one day of the simulation period as well as the development of stagnation and episodic conditions in the Northeast U.S.

3.1.2 NEROS/PEPE Data Bases

During the 1980 summer season EPA's Office of Research and Development sponsored two major field studies in the Northeast U.S. The first was the Northeast Regional Oxidant Study (NEROS), (Vaughan, 1985). The NEROS field measurements concentrated on sampling strategies to clarify and parameterize essential

processes simulated within the ROM, to provide input data for the model, and to provide data with which to evaluate the model. While some special study measurements were made at the surface as part of the NEROS, especially for non-methane hydrocarbons (NMHC), most of the measurements were obtained by aircraft. The aircraft flights were both of regional nature (long horizontal flight tracks) and of local nature (spirals and transects within and near urban and power plant plumes). Generally, instrumentation on board the several aircraft used during the NEROS continuously measured O_3 , NO_2 , and NO_x , and intermittent grab samples of NMHC were obtained for later analysis.

The Persistent Elevated Pollutant Episode (PEPE) study was performed in conjunction with the NEROS in 1980. Its focus was on a regional perspective concerning the broad regions of haze associated with large stagnant air masses. The interrelationships between the emissions of sulfur and nitrogen oxides from large power plants and regional haze was a key concern, and aircraft monitoring in this study concentrated on following urban and power plant plumes into the regional environment. Aircraft were based in Columbus, OH for the NEROS and PEPE experiments and in Baltimore, MD for Baltimore plume studies conducted as part of NEROS.

3.1.3 NECRMP

The Northeast Corridor Regional Modeling Program (NECRMP), sponsored by EPA's Office of Air Quality Planning and Standards (Possiel and Freas, 1982), included urban field studies during the summer of 1980 designed to collect the necessary air quality and meteorological data necessary to apply the Urban Airshed Model (Ames *et al.*, 1985) to Washington, DC, Baltimore, New York, and Boston. The data requirements for applying and evaluating this model led to the development of a monitoring program including air quality measurements by aircraft upwind of the urban area in the morning, and over and downwind of the urban area in the afternoon. The aircraft measurements included O_3 , NO_2 , NO_x , and NMHC. Special surface measurements of NMHC were also obtained in each urban area in the 06-09 h, LDT time period.

Monitoring flights were conducted on days when photochemical activity and subsequent widespread high O_3 concentrations would be likely. The flight plans included vertical spirals and horizontal transects designed to map the pollutant concentration fields aloft. Transects were flown at ≈ 750 m above ground level, with spirals from 150-2100 m over rural areas and 300-2100 m over urban areas.

3.1.4 Emissions

There are two major components to the emissions inventory data base needed by the ROM system: the anthropogenic emissions, and the biogenic emissions. Anthropogenic emissions of NO_x , CO, and various categories of NMHC were obtained from the 1980 National Acid Precipitation Assessment Program (NAPAP) emissions inventory (Wagner *et al.*, 1986). The NAPAP version 5.0 annual inventory spans the 48 contiguous states and 10 Canadian provinces, providing detailed point source data for over 14,000 plants and area source information by source category for 3070 U.S. counties and 10 Canadian provinces. The transition from the annual inventory to the hourly gridded inventory used in the ROM was accomplished using the Flexible Regional Emissions Data System (FREDS). Temporal, spatial, and species allocation factors were developed and used by FREDS to process the annual NAPAP inventory into the NAPAP version 5.3 inventory used by the ROM in this application. The final inventory contains hourly emission rates on the ROM's 18.5-km grid resolution for NO, NO_2 , CO, and the NMHC categories of ethylene, olefins, paraffins, formaldehyde, higher aldehydes, toluene, xylene, and non-reactives.

The biogenic portion of the emissions inventory consists of hourly, gridded values of natural hydrocarbon species. This inventory was developed at EPA (Novak and Reagan, 1986). Three basic components are required to develop estimates of hourly, gridded biogenic NMHC emissions: (a) emission factors representative of vegetative species indigenous to the modeling region, (b) empirical relationships between emission factors and specific environmental parameters, and (c) quantitative estimates of vegetation density of the representative species in a designated area. The development of the biogenic inventory consisted of the compilation and assimilation of each of these factors. Biogenic NMHC emissions for an individual vegetative species, then, are estimated by multiplying an hourly emission factor by the individual species biomass. Total emissions per grid cell is the sum of the individual vegetative species emissions. The resulting biogenic inventory consists of estimates of isoprene, monoterpenes, and methane. For use in the ROM, isoprene emissions are used directly, while monoterpenes are divided between the olefin and paraffin classes.¹ Natural methane emissions are not assimilated by the ROM system; rather, a constant background methane concentration of 1.85 ppm is implicitly included in the appropriate reactions of the ROM's chemical kinetic mechanism.

A comparison of the magnitudes of total NMHC between the anthropogenic and biogenic inventories shows that for major urban areas the anthropogenic component is far larger than the biogenic component. For the overall ROM region in the Northeast U.S. however, the integrated anthropogenic NMHC emissions rate, over the modeling domain was 1.7×10^7 kg/day and the total biogenic NMHC emissions rate, including unidentified compounds, was 2.6×10^7 kg/day for a mid-summer day

¹ 1 mole monoterpenes = 1 mole olefins + 8 moles paraffins

with clear skies. These figures encompass an emissions area of 1 million km². If the non-reactive components are excluded from the anthropogenic emissions rate and the unidentified compounds are excluded from the biogenics emissions rate, the ratio of biogenic emissions to anthropogenic emissions becomes 1.2:1. This ratio reflects the organic emissions as they influence oxidant chemistry in the ROM.

3.2 INITIAL AND BOUNDARY CONCENTRATIONS

Providing an initial field of concentration values for a regional model is a very difficult problem. There are insufficient monitoring data, even under special field study conditions, to adequately specify a gridded concentration field for all required species. Initial attempts at using air quality data to provide initialization for ROM1.0 model applications showed that errors in the mass loading of the initial field led to artifacts in the model simulation for the first 24–36 hours. Eventually the initial field is effectively transported out of the model domain. To circumvent the initialization problem, the ROM is initialized on a relatively clean day several days before any periods of high O₃ concentrations are found to exist in the domain. The full domain is assumed to contain spatially invariant values of clean tropospheric background concentrations of O₃, NO_x, and NMHC.² These species concentrations were then allowed to chemically equilibrate, using an independent chemical solution module containing the same chemical kinetics mechanism used in ROM2.0, for a 10-h period in full-sun conditions. The resulting set of species concentrations, shown in Table 3.1, were used for initial values. The set of initial values was spatially invariant in each horizontal model layer, but contained small vertical variations dependent on the photolysis rate gradient in the vertical as determined by the solar radiation profile. To further isolate the model results from initial condition artifacts, the results for the first 24 hours of simulation are not used in the model evaluation analysis.

Hourly boundary concentrations for all species are required by the ROM along all borders of the domain during the simulation. The same scarcity of data plaguing the initial condition problem also makes determining the boundary conditions difficult. As mentioned above, most surface monitoring sites are located in or near urban areas and are not representative of large areas of the ROM domain. Aircraft measurements are more useful in this regard, but they are sporadic and not made on the same time scales as the ROM requires.

The boundary condition problem cannot be circumvented in the same manner as the initial condition problem. The goal, therefore, is to mitigate the effect of the boundary conditions. This has been done to some extent by the specification of the size of the model domain. While the area of greatest interest in the simulations

²Clean tropospheric background values used are: O₃=35 ppb, NO_x=2 ppb, NMHC=15 ppb.

TABLE 3.1. INITIAL EQUILIBRATED CONCENTRATIONS FOR ROM2.0
(LAYER 1)

Species	Conc. (ppb)	Species	Conc. (ppb)	Species	Conc. (ppb)
ALD2	9.0×10^{-2}	MGLY	1.5×10^{-3}	PAN	5.2×10^{-2}
C2O3	7.4×10^{-4}	N2O5	1.7×10^{-6}	PAR	3.2
CO	9.9×10^2	NO	5.1×10^{-2}	PHEN	4.3×10^{-2}
ETH	1.7×10^{-2}	NO2	1.5×10^{-1}	PHO	4.1×10^{-6}
FORM	1.1	NO3	2.0×10^{-5}	TLA	9.3×10^{-6}
H2O2	1.1	NONR	1.0×10^{-13}	TOL	1.2×10^{-2}
HNO2	1.9×10^{-3}	O	1.5×10^{-7}	XO2	1.2×10^{-2}
HNO3	1.6	O3	3.2×10^1	XO2N	1.4×10^{-3}
HO2	2.5×10^{-2}	OH	2.9×10^{-4}	XYL	1.3×10^{-6}
ISOP	1.0×10^{-13}	OLE	4.7×10^{-6}		

is in the Northeast Corridor from Washington through Boston, the model domain extends in an upwind direction to the Ohio Valley and south to northern Virginia and West Virginia. In this way the model assimilates all of the significant upwind sources potentially making an impact on the Northeast Corridor and thereby reducing the influence of boundary conditions in that area. Obviously, the farther west and south in the domain one goes from the Corridor, the greater will be the boundary condition influence.

As a starting point, we have assumed the same tropospheric background conditions at the ROM boundaries as were described for the initial conditions, with one exception. We allow for the fact that O_3 may deviate from this background value at lateral boundaries. At best, we have identified three upwind SAROAD sites that are in relatively rural locations and may be used as regionally representative monitors. There is one station each in Ohio, Virginia, and West Virginia. The data at these stations were averaged in the 1000–1600 h, LST block and the 2200–0400 h block to determine representative daytime and nighttime O_3 values, respectively, at each station. Then the average over the three stations was computed. Table 3.2 lists the O_3 values computed for each day of the simulation period in this manner.

For a given day and time period the same O_3 value was used at all lateral boundaries. The set of chemically equilibrated clean tropospheric background concentrations, used for initial conditions, was re-equilibrated for 90 minutes using the specified boundary O_3 value. The re-equilibrated concentrations were then used at all lateral boundaries for a ≈ 12 hour period. The O_3 value was updated from day to night, and night to day conditions. A nighttime set of tropospheric chemically

equilibrated concentrations was formed to use in conjunction with the nighttime O_3 values. The chemical equilibration step is needed to save the ROM from performing the same equilibration in every boundary grid cell (or in every grid cell, for the case of initial conditions) during simulation.

ROM layer 1 boundaries use the daytime O_3 value (and other daytime values of the remainder of the equilibrated species) during the period 0700–2000 h and the nighttime O_3 value (and other nighttime values of the remainder of the equilibrated species) during the period 2000–0700 h. For layers 2 and 3, where the observed nighttime O_3 values at the surface are not as relevant, the daytime O_3 (and other species' daytime equilibrated values) are used during the daytime period, and the next daytime O_3 value (and other species nighttime equilibrated values) are used during the nighttime period. The rationale for using the next day's O_3 value for nighttime in layers aloft is based on the faster transport of material in layers above the surface and the isolation of the O_3 contained in this material from surface sources of NO_x scavenging.

TABLE 3.2. UPWIND O₃ BOUNDARY CONCENTRATIONS

Date	Julian Date	Day (ppb)	Night (ppb)	Date	Julian Date	Day (ppb)	Night (ppb)
July 12	80194	70	33	Aug. 6	80219	43	21
July 13	80195	52	20	Aug. 7	80220	44	34
July 14	80196	55	18	Aug. 8	80221	52	21
July 15	80197	54	15	Aug. 9	80222	56	28
July 16	80198	63	19	Aug. 10	80223	60	30
July 17	80199	62	21	Aug. 11	80224	68	40
July 18	80200	64	21	Aug. 12	80225	57	20
July 19	80201	65	19	Aug. 13	80226	62	18
July 20	80202	57	18	Aug. 14	80227	62	19
July 21	80203	44	17	Aug. 15	80228	55	34
July 22	80204	38	25	Aug. 16	80229	37	28
July 23	80205	42	24	Aug. 17	80230	31	20
July 24	80206	61	23	Aug. 18	80231	41	24
July 25	80207	66	30	Aug. 19	80232	46	27
July 26	80208	58	49	Aug. 20	80233	57	23
July 27	80209	65	34	Aug. 21	80234	54	39
July 28	80210	35	28	Aug. 22	80235	47	29
July 29	80211	61	36	Aug. 23	80236	53	22
July 30	80212	46	28	Aug. 24	80237	55	15
July 31	80213	69	32	Aug. 25	80238	55	13
Aug. 1	80214	63	27	Aug. 26	80239	68	17
Aug. 2	80215	69	53	Aug. 27	80240	70	17
Aug. 3	80216	60	31	Aug. 28	80241	74	19
Aug. 4	80217	55	21	Aug. 29	80242	71	24
Aug. 5	80218	50	20	Aug. 30	80243	54	25
				Aug. 31	80244	54	-

4 MODEL EVALUATION

Model evaluation is an elusive concept. In broad terms it consists of testing a model with a historical data set of known accuracy and carefully comparing model predictions with these observed data. In classical experimentation, models are tested in isolated environments to minimize the influence of external factors. For models of the atmosphere this type of testing is not possible. Air pollution models are driven by meteorological, air quality, and emissions data whose accuracy is not well established. Results of these models are compared with historical data whose spatial and temporal scales of representativeness are often different than those of the model results. The methods of comparing these disparate data sets and the meaning ascribed to the comparisons contain as much art as they do science. Because of the inability to control all of the degrees of freedom in air quality model evaluation experiments there are as many methods to evaluate a model as there are model evaluators. The common thread among all evaluations of air quality models is a desire to establish the credibility of the model at properly simulating the physical and chemical processes responsible for the transport, transformation, and fate of air pollutants. The second common need is to establish the strengths and limitations of the model for setting caveats and guidance regarding the model's use.

There is a further complication in (air quality) model evaluation. It may be possible to evaluate a model for a given set of input data representing some base state. It is, however, not currently possible to evaluate a model from the base state to some future state. For example, models of photochemical air pollution, like the ROM, are used to help assess the degree of precursor emission control required to bring the maximum O_3 concentrations to the level of the national standard (120 ppb). Therefore, what the air quality policy analyst is really interested in is not necessarily the model's ability to predict the maximum O_3 concentration from a historical data set, but rather to predict $\partial O_3 / \partial S$, where S is the source emissions term. Correct estimation of the absolute O_3 concentrations may be a necessary condition for this, but it is not sufficient. Unfortunately, existing data bases, particularly for source emissions, are inadequate for assessing $\partial O_3 / \partial S$ from ambient

or model-simulated data bases. Therefore, the type of evaluation we perform will provide part, but not all, of the evidence needed to establish credibility for usefulness of the model as a tool by the model users in the regulatory community. As higher quality emission inventories with less inherent uncertainty become available, and consistent procedures are employed in developing these inventories so that a coherent temporal emissions history is available, we may be able to perform the definitive type of model evaluation that is required.

It is useful to contrast the often confused concepts of model evaluation and model *validation*. Evaluation is not the same as validation in this context. A valid model is one in which the requisite physical and chemical processes have been adequately included and correctly represented in the simulation process. For example, the chemical representation of photochemical smog processes should have been simulated with an up-to-date kinetic mechanism that has been separately evaluated with smog chamber experimental data. The transport mechanism should have been tested against analytic flow representations with exact solutions as well as perhaps tracer experiments in the atmosphere. An evaluated model is one in which the entire simulation "package" or model has successfully been tested against ambient observational data, such as maximum O₃ concentrations. It is possible for a valid model to perform poorly in atmospheric simulations, just as it is possible for a highly empirical model to perform well.

How, then, do we proceed to evaluate the ROM? A preliminary attempt was made with the first generation model, ROM1.0, when the results from a two day episode were compared to 1979 NEROS surface and aircraft data (Schere, 1986). The methods used in that analysis were largely deterministic. That is, the model concentration predictions for a specific location are compared to observations taken at that location on a given day. Historically, most air quality model evaluations have been performed deterministically. Lamb (1984) maintains that there are inherent limitations on the predictability of air quality models, particularly on regional and larger spatial scales. He suggests that, even if the model is formulated perfectly, the data needed to drive the model are not sufficient to exactly determine the state of the atmosphere. This uncertainty in the atmospheric state gives rise to corresponding uncertainties in the concentration predictions from even a perfect model. The magnitude of the uncertainties in the concentration values is directly proportional to the extent to which concentrations at a receptor are affected by distant sources. Furthermore, the level of uncertainty increases with increasing distance from the nearest meteorological station and with increasing distance to significant sources.

Lamb's ideas concerning the uncertainty in atmospheric state translate directly into uncertainty in the wind-driven transport component of the air quality model solution. Consider, for example, that wind fields used to drive air quality models are typically derived from some sort of objective interpolation of existing

meteorological data. Upper air wind monitoring data are a necessary component of this meteorological data set. However, upper air monitoring stations are located 300–500 km apart in the U.S. The number of these stations used in a wind field calculation for a 1000-km domain therefore would vary between 4 and 12. Consequently, one upper air measurement station would determine the wind pattern over a square horizontal area 300 km on a side under the best circumstances, and 500 km on a side under the worst. By comparison, the horizontal spatial resolution required in the ROM is 18.5 km. When objective analysis techniques are applied to these wind data to determine spatially gridded wind field patterns, the results in the vicinity of wind monitoring stations would appear nearly the same no matter which analysis technique was chosen. However, as distance away from the monitoring station increases, more variations will appear in the analyzed wind fields from one technique to another. This is the “inherent uncertainty in atmospheric state” that Lamb discusses. The predictability of a model therefore decreases with increasing distance of sources and/or receptors from meteorological stations. In other words, the ability to attribute pollutant levels in remote regions to specific sources is inherently limited. Thus the predictions even of a perfect model cannot be expected to agree with observations at all locations.

Lamb and Hati (1987) propose a method for generating an ensemble, C , of possible wind fields that are applicable for use in regional scale air quality models from one set of meteorological observations. This concept explicitly addresses the uncertainty inherent in the specification of atmospheric states. From the ensemble, C , one can specify the frequency with which the actual concentration can be expected to fall within a given interval of values in a large number of observations. The width of this interval is a measure of the “predictability” of the concentration and it is determined by the properties of the set, C . The application of this concept for regional air quality models takes them from a deterministic mode to a *probabilistic* mode in which the prediction of the pollutant concentration at a receptor is in the form of an expected probability distribution. Lamb (1984) then defines the goal of model evaluation to be that of determining whether observed concentrations fall within the interval indicated by the model with the frequency indicated, and if not, whether the failure is attributable to sampling fluctuations or is due to the failure of the hypotheses on which the model is based. From the standpoint of regulatory users, the utility of a model can then be measured partly by the width of the interval in which a majority of the observations can be expected to fall. If the width of the interval is very large, the model may provide no more information than one could gather simply by guessing the expected concentration. In other words, when the width of the interval of probable concentration values exceeds the allowable error bounds on the model's predictions, the model is of no value in that particular application. As discussed, the widest intervals are expected to be at those receptors most distant from both sources and meteorological monitoring stations.

The implementation of the concept of Lamb's probabilistic wind fields has, unfortunately, proved to be very difficult and will not be a reality within the near future. Alternatively, we use a concept in this evaluation study which remains true to the probabilistic mode in that model predictions and observations are not compared for a specific location and time. However, instead of aggregating model predictions of simulations at a specific receptor location using various wind field "realizations", we will aggregate concentrations at groups of receptor locations and compare the aggregate frequency distribution of concentrations from the receptor group with that of the observed concentrations from the group. In an operational sense this method of aggregating modeling results assumes that the wind field's inherent uncertainty is one of the largest potential sources of error in the model results. Aggregation over space and time consequently assumes that, if these transport errors are more or less randomly distributed, the errors they produce in model predictions will compensate when one takes a broad space and time perspective on matching predictions and observations. Specific methods of aggregating stations are discussed in the sections that follow. Lamb terms this method of evaluation as "quasi-deterministic", and is an interim method to be used only until the full probabilistic concept can be implemented.

In the analyses that follow we use the quasi-deterministic mode for the evaluation of ROM results when comparing predictions to surface-monitored observations of O_3 , NO_2 , and NO_x . This is possible because there are sufficient numbers of these monitoring stations to form coherent groups for the aggregation step in the analysis. For surface monitoring of NMHC and also for all aircraft monitoring there are not sufficient stations, or, in the case of aircraft, the data are obtained too intermittently, to form groups for aggregation. It is therefore more difficult to implement the quasi-deterministic method of evaluation. In this case we form the most appropriate spatial and/or temporal averages of data to compare with observations. Usually, however, there is a fundamental difference in the spatial or temporal scales of the observed and the predicted data. Therefore, in these cases, our comparisons are less quantitative and more descriptive because we run the risk of inappropriate comparisons, or the often-described comparison of "apples and oranges". As we make more such *diagnostic* comparisons, however, the complete picture of model performance comes into focus. For the surface analyses of O_3 , NO_2 , and NO_x , where the analysis adheres more strictly to the quasi-deterministic mode, we employ quantitative comparisons of observed and predicted data using descriptive statistics as well as graphical analyses. The combination of quantitative comparison of observed and predicted data of similar scale and the qualitative comparison of observed and predicted data of dissimilar scale was thought to be the most appropriate combination for use in the ROM evaluation. With this combination we attempt to maintain a balance of the use of all available data with the conscious desire to use the data *appropriately*. In this context, the rigorous comparison of data of dissimilar scales is considered inappropriate. In the sections that follow, the specific analyses on per-

formance evaluation of the ROM for surface-observed O_3 , NO_2 , NO_x , and NMHC, and aircraft-observed O_3 , NO_x , and NMHC are described.

5 EVALUATION OF SURFACE-BASED O₃

5.1 DATA PREPARATION

5.1.1 Surface Monitoring Network

The SAROAD and Canadian surface O₃ monitoring data base contained 214 individual sites that were active during some or all of the simulation period studied. Hourly average O₃ concentrations were available from these sites. Most of the sites in the surface network were located within or near urban areas. As a result there is good spatial coverage in selected portions of the ROM domain and poor spatial coverage in much of the remainder of the domain. Figure 5.1 shows the grid cells within the ROM domain containing at least one surface O₃ monitoring station and Table 5.1 lists each of the stations and their locations. Generally, for those cells that contained monitors, there was no more than one site per cell. Several cells, however, in major urban areas contained multiple monitoring sites.

Some of the urban-oriented monitors often show the effects of local NO_x scavenging of O₃, especially during the nighttime hours. Nevertheless, the large number of monitors and the extended simulation period provide useful data for performing an evaluation of the ability of the ROM to simulate O₃ concentrations over regional scales. Our discussion in this section is limited to the performance of the model for predicting O₃ near ground level only.

5.1.2 Frequency and Cluster Analysis

The evaluation of surface-based O₃ concentrations here will follow along the lines of the quasi-deterministic analysis discussed previously. We will focus on the ability of the ROM to simulate O₃ concentration frequency distributions at groups of receptor locations during the simulation period. Each group of receptors shall have

TABLE 5.1. OZONE MONITORING STATIONS - NEROS REGION - 1980

I.D.	Location	State	Lat. (deg.,N)	Lon. (deg.,W)	ROM Grid Cell	
					x	y
BR2	BRIDGEPORT	CT	41.1867	73.1764	44	20
DAN	DANBURY	CT	41.4014	73.4447	43	21
DRB	DERBY	CT	41.3164	73.0878	44	20
GRW	GREENWICH	CT	41.0794	73.7053	42	19
HF2	HARTFORD	CT	41.7608	72.6789	46	23
LCH	LITCHFIELD CO	CT	41.6725	73.1431	44	23
MDL	MIDDLETOWN	CT	41.5519	72.6308	46	22
NH2	NEW HAVEN	CT	41.3078	72.9233	45	20
STF	STAFFORD	CT	41.9758	72.3867	47	24
STR	STRATFORD	CT	41.1528	73.1511	44	19
DC1	WASHINGTON	DC	38.9036	77.0517	28	6
DC2	WASHINGTON	DC	38.9753	77.0228	28	6
DOV	DOVER	DE	39.1486	75.5000	35	7
NC1	NEW CASTLE CO	DE	39.8083	75.4500	35	11
NC2	NEW CASTLE CO	DE	39.7750	75.5167	34	11
NC4	NEW CASTLE CO	DE	39.5333	75.6864	34	10
SUS	SUSSEX CO	DE	38.5842	75.2736	35	4
AS1	ASHLAND	KY	38.4436	82.6131	6	3
AGA	AGAWAM	MA	42.0356	72.6358	46	25
ATL	ATTLEBORO	MA	41.9300	71.2650	51	24
BS3	BOSTON	MA	42.3781	71.0283	52	27
CHR	CHARLTON	MA	42.3128	71.9653	49	26
DVR	DANVERS	MA	42.5919	70.9769	53	28
EST	EASTON	MA	42.0672	71.0906	52	25
GRG	GEORGETOWN	MA	42.7239	70.9869	53	29
HAM	HAMILTON	MA	42.6306	70.8153	53	28
MED	MEDFIELD	MA	42.2122	71.3356	51	26
MNT	MONTAGUE	MA	42.5669	72.5283	46	28
PTS	PITTSFIELD	MA	42.4525	73.2011	44	27
QIN	QUINCY	MA	42.2444	70.9719	53	26
SOM	SOMERVILLE	MA	42.4036	71.1083	52	27
SDB	SUDBURY	MA	42.3850	71.3889	51	27
TEW	TEWKSBURY	MA	42.6081	71.2206	52	28
WAT	WATERTOWN	MA	42.3747	71.1825	52	27
W01	WORCESTER	MA	42.2586	71.8006	49	26
W02	WORCESTER	MA	42.3000	71.7500	50	26
AA2	ANNE ARUNDEL CO	MD	39.1697	76.6278	30	8
AA3	ANNE ARUNDEL CO	MD	38.9028	76.6528	30	6
AA4	ANNE ARUNDEL CO	MD	39.1014	76.7278	30	7
BL1	BALTIMORE	MD	39.2997	76.6131	30	8
BL2	BALTIMORE	MD	39.2367	76.5844	30	8
BL3	BALTIMORE	MD	39.3147	76.6142	30	8
BL6	BALTIMORE CO	MD	39.4058	76.7653	29	9
BL7	BALTIMORE CO	MD	39.5150	76.4311	31	10
CCL	CECIL CO	MD	39.7186	76.1061	32	11
CKY	COCKEYSVILLE	MD	39.4611	76.6311	30	9
DMS	DAMASCUS	MD	39.2744	77.2214	28	8
EDG	EDGEWOOD	MD	39.4097	76.2972	31	9
ESX	ESSEX	MD	39.3531	76.4814	31	9
FRD	FREDERICK CO	MD	39.4797	77.2319	28	9
GRN	GREENBELT	MD	39.0200	76.8278	29	7

TABLE 5.1. (continued)

HRF	HARFORD CO	MD	39.6269	76.3294	31	10
RVB	RIVIERA BEACH	MD	39.1597	76.5117	30	7
RCK	ROCKVILLE	MD	39.1133	77.1072	28	7
SUT	SUITLAND-SILVER HILL	MD	38.8533	76.9319	29	6
CPE	CAPE ELIZABETH	ME	43.5658	70.2000	56	34
CUM	CUMBERLAND CO	ME	43.9086	70.2306	56	36
GRD	GARDINER	ME	44.2250	69.7906	57	38
ALP	ALLEN PARK	MI	42.2286	83.2103	4	26
DT2	DETROIT	MI	42.3583	83.0975	4	27
DT3	DETROIT	MI	42.4333	83.0036	4	27
ESS	ESSEXVILLE	MI	43.6156	83.8453	1	34
FLN	FLINT	MI	43.0247	83.6858	2	31
GNS	GENESEE CO	MI	43.1683	83.4617	3	32
LIV	LIVONIA	MI	42.3819	83.4039	3	27
MAC	MACOMB CO	MI	42.7247	82.7917	5	29
PRH	PORT HURON	MI	42.9478	82.4417	7	30
SAL	SALINE	MI	42.1556	83.7781	1	25
STH	SOUTHFIELD	MI	42.4539	83.2194	4	27
WRN	WARREN	MI	42.5133	83.0061	4	28
MN1	MANCHESTER	NH	42.9928	71.4644	51	30
PO1	PORTSMOUTH	NH	43.0781	70.7628	53	31
AC1	ATLANTIC CO	NJ	39.5247	74.4597	39	10
BAY	BAYONNE	NJ	40.6811	74.1197	40	17
CM1	CAMDEN	NJ	39.9231	75.0972	36	12
CM3	CAMDEN CO	NJ	39.6739	74.8569	37	11
CPM	CAPE MAY CO	NJ	39.1036	74.8150	37	7
DUM	DUMONT	NJ	40.9378	73.9950	41	18
ESO	EAST ORANGE	NJ	40.7564	74.2006	40	17
FLM	FLEMINGTON	NJ	40.5167	74.8100	37	16
LIN	LINDEN	NJ	40.6044	74.2533	39	16
MCG	MC GUIRE AFB	NJ	40.0486	74.5839	38	13
MON	MONMOUTH CO	NJ	40.3278	74.2667	39	14
MRC	MORRIS CO	NJ	40.7878	74.6775	38	17
NWR	NEWARK	NJ	40.7328	74.1781	40	17
NWB	NEW BRUNSWICK	NJ	40.4822	74.4408	39	15
PLN	PLAINFIELD	NJ	40.6011	74.4419	39	16
SHV	SOMERVILLE	NJ	40.5694	74.6136	38	16
TRN	TRENTON	NJ	40.2200	74.7650	37	14
VIN	VINELAND	NJ	39.4922	75.0208	36	9
AMH	AMHERST	NY	42.9925	78.7764	21	30
BAB	BABYLON	NY	40.7356	73.4061	43	17
BNG	BINGHAMTON	NY	42.0994	75.8936	33	25
ELM	ELMIRA	NY	42.1094	76.8022	29	25
EXC	ESSEX CO	NY	44.3650	73.9017	41	39
GLN	GLENS FALLS	NY	43.3167	73.6239	42	32
HM1	HEMPSTEAD	NY	40.7453	73.5869	42	17
HM2	HEMPSTEAD	NY	40.8917	73.5986	42	18
MAM	MAMARONECK	NY	40.9314	73.7639	41	18
MNR	MONROE CO	NY	43.0733	77.7108	26	31
NY2	NEW YORK CITY	NY	40.7358	73.8169	41	17
NY4	NEW YORK CITY	NY	40.5925	73.9375	41	16
NY5	NEW YORK CITY	NY	40.7394	73.9861	41	17
N10	NEW YORK CITY	NY	40.5972	74.1264	40	16
N11	NEW YORK CITY	NY	40.7775	73.9086	41	17
N12	NEW YORK CITY	NY	40.6719	73.9778	41	17

TABLE 5.1. (continued)

NG1	NIAGARA CO	NY	43.2189	78.4792	23	32
NG2	NIAGARA FALLS	NY	43.0858	78.9964	21	31
ONI	ONEIDA CO	NY	43.3039	75.7214	34	32
POU	POUGHKEEPSIE	NY	41.7033	73.9356	41	23
REN	RENSSELAER	NY	42.6275	73.7511	41	28
RC2	ROCHESTER	NY	43.1669	77.5169	26	32
SCH	SCHENECTADY	NY	42.7964	73.9394	41	29
SYB	STONY BROOK	NY	40.9125	73.1292	44	18
SY1	SYRACUSE	NY	43.0453	76.1478	32	31
SY3	SYRACUSE	NY	43.0600	76.1267	32	31
UTC	UTICA	NY	43.0997	75.1967	36	31
WAY	WAYNE CO	NY	43.2303	77.1728	28	32
WPL	WHITE PLAINS	NY	41.0522	73.7642	41	19
AK2	AKRON	OH	41.1061	81.5033	10	19
BAR	BARBERTON	OH	40.9986	81.6311	10	18
BER	BEREA	OH	41.3714	81.8536	9	21
CAN	CANTON	OH	40.7975	81.3750	11	17
CLK	CLARK CO	OH	40.0011	83.8044	1	13
CL2	CLEVELAND	OH	41.5547	81.5744	10	22
CLN	CLINTON CO	OH	39.4272	83.7872	1	9
CB1	COLUMBUS	OH	40.0000	83.0417	4	13
CB4	COLUMBUS	OH	39.9622	82.9925	5	12
CB5	COLUMBUS	OH	40.0869	82.9603	5	13
CNE	CONNEAUT	OH	41.9594	80.5725	14	24
EY2	ELYRIA	OH	41.3661	82.1083	8	21
LOG	LOGAN	OH	39.5272	82.3758	7	10
MAH	MAHONING CO	OH	41.1147	80.9828	13	19
MDN	MEDINA CO	OH	41.1547	81.9028	9	19
PAI	PAINESVILLE	OH	41.7217	81.2428	12	23
PTG	PORTAGE CO	OH	41.1822	81.3303	11	20
STK	STARK CO	OH	40.8708	81.3308	11	18
STU	STEUBENVILLE	OH	40.3594	80.6231	14	15
TL1	TOLEDO	OH	41.6472	83.5300	2	22
TL4	TOLEDO	OH	41.7181	83.4758	3	23
WSL	WESTLAKE	OH	41.4753	81.8794	9	21
YG2	YOUNGSTOWN	OH	41.0997	80.6503	14	19
HRP	HURON PARK, ONT	ON	43.2913	81.4931	11	32
WNS	WINDSOR, ONT	ON	42.3160	83.0434	4	26
MRL	MERLIN, ONT	ON	42.2457	82.2230	8	26
SR2	SARNIA, ONT	ON	42.9785	82.4054	7	30
PTR	PETROLIA, ONT	ON	42.9557	82.1928	8	30
CR3	CORUNNA, ONT	ON	42.9130	82.4529	7	30
LND	LONDON, ONT	ON	42.9896	81.2232	12	30
TV2	TIVERTON, ONT	ON	44.3012	81.5754	10	38
SMC	SIMCOE, ONT	ON	42.8560	80.2693	15	30
LPT	LONG POINT PARK, ONT	ON	42.5766	80.3883	15	28
BNW	BINBROOK WEST, ONT	ON	43.1203	79.8765	17	31
KCH	KITCHENER, ONT	ON	43.4578	80.4722	15	33
STC	ST. CATHERINES, ONT	ON	43.1654	79.2397	20	31
HML	HAMILTON, ONT	ON	43.2586	79.8432	17	32
TR1	TORONTO, ONT	ON	43.6601	79.3878	19	34
TR2	TORONTO, ONT	ON	43.6472	79.3671	19	34
SCR	SCARBOROUGH, ONT	ON	43.7485	79.2749	19	35
NYK	NORTH YORK, ONT	ON	43.7197	79.3390	19	35
EB1	ETOBICOKE, ONT	ON	43.6501	79.5840	18	34

TABLE 5.1. (continued)

EB2	ETOBICOKE, ONT	ON	43.6169	79.5228	18	34
BLG	BURLINGTON, ONT	ON	43.3158	79.8014	17	32
OK2	OAKVILLE, ONT	ON	43.4174	79.6993	18	33
OSH	OSHAWA, ONT	ON	43.8962	78.8535	21	36
MSG	MISSISSAUGA, ONT	ON	43.5703	79.6106	18	34
STV	STOUFFVILLE, ONT	ON	43.9663	79.2661	19	36
AG1	ALLEGHENY CO	PA	40.3819	80.1856	16	15
AG2	ALLEGHENY CO	PA	40.4367	79.9544	17	15
AG3	ALLEGHENY CO	PA	40.4428	79.9881	17	15
AG4	ALLEGHENY CO	PA	40.4722	79.8200	17	15
ALN	ALLENTOWN	PA	40.6186	75.4489	35	16
BAD	BADEN	PA	40.6356	80.2308	16	16
BVF	BEAVER FALLS	PA	40.7478	80.3167	15	17
BET	BETHLEHEM	PA	40.6203	75.3644	35	16
BCK	BRACKENRIDGE	PA	40.6108	79.7464	18	16
BRI	BRISTOL (BOROUGH)	PA	40.2475	74.9972	37	14
CHL	CHARLEROI	PA	40.1469	79.9033	17	13
CHT	CHESTER	PA	39.8369	75.3747	35	12
CNS	CONSHOHOCKEN	PA	40.0719	75.2992	35	13
EAS	EASTON	PA	40.6761	75.2175	36	17
ERE	ERIE	PA	42.1394	80.0467	16	25
HAR	HARRISBURG	PA	40.2444	76.8472	29	14
JNS	JOHNSTOWN	PA	40.3097	78.9158	21	14
KUT	KUTZTOWN	PA	40.5108	75.7853	33	16
LAN	LANCASTER CITY	PA	40.0439	76.2867	31	13
MDD	MIDLAND	PA	40.6350	80.4444	15	16
NCL	NEW CASTLE	PA	40.9958	80.3467	15	18
NRS	NORRISTOWN	PA	40.1122	75.3106	35	13
PRY	PERRY CO	PA	40.4578	77.1675	28	15
PH2	PHILADELPHIA	PA	40.0500	75.2406	36	13
PH6	PHILADELPHIA	PA	39.9078	75.1494	36	12
PH7	PHILADELPHIA	PA	40.0764	75.0119	36	13
PT2	PITTSBURGH	PA	40.4656	79.9611	17	15
RDG	READING	PA	40.3208	75.9278	33	14
SC1	SCRANTON	PA	41.4431	75.6244	34	21
SC2	SCRANTON	PA	41.5917	76.0722	32	22
WLK	WILKES-BARRE	PA	41.2378	75.8958	33	20
YOR	YORK	PA	39.9656	76.6992	30	12
KNT	KENT CO	RI	41.6150	71.7197	50	22
PV4	PROVIDENCE	RI	41.8256	71.4053	51	23
ALX	ALEXANDRIA	VA	38.8106	77.0447	28	5
ARL	ARLINGTON CO	VA	38.8575	77.0592	28	6
FX1	FAIRFAX	VA	38.8447	77.3119	27	6
FX3	FAIRFAX CO	VA	38.7422	77.0775	28	5
FDR	FREDERICKSBURG	VA	38.3111	77.4489	27	2
MCL	MC LEAN	VA	38.9344	77.1983	28	6
PWM	PRINCE WILLIAM CO	VA	38.6419	77.5283	26	4
SVC	SEVEN CORNERS	VA	38.8678	77.1431	28	6
BU1	BURLINGTON	VT	44.4789	73.2119	44	39
BU2	BURLINGTON	VT	44.4567	73.1939	44	39
GMT	GREEN MOUNTAIN NAT.	VT	43.9333	73.0333	44	36
CHS	CHARLESTON	WV	38.3419	81.6200	10	3
WH2	WHEELING	WV	40.1206	80.6997	14	13

certain characteristics common to all members of the group. In our case we have chosen the observed frequency distribution of O_3 concentrations to be the common characteristic. The first step toward forming coherent groups of stations was to do a histogram-type analysis on the observed concentrations from the monitors in the surface network over the model simulation period. Concentration ranges for the histogram analysis were chosen as follows¹:

5 - 20 ppb Concentrations in this range are unusually low; probably affected by NO_x scavenging from local sources.

5 - 40 ppb Concentrations in this range are within tropospheric background limits. This range overlaps the first range; each represents a distinct and *different* mode of classification based on historical O_3 concentration patterns.

40 - 80 ppb Concentrations in this range indicate low O_3 production.

> 80 ppb Concentrations in this range show a moderate to high degree of O_3 production.

Only daytime (0800–1900 h, LST) hourly values were included in the histogram analysis. The ROM's diagnostic surface layer is not yet operational and thus is unable to predict actual surface concentrations. Consequently we are using model predictions from model layer 1, which is typically 100–500 m deep and most closely represents the surface layer under well-mixed conditions such as occur during the day. Titration of O_3 by surface NO_x sources and ground deposition can cause larger vertical gradients at night. At this time the ROM's layer 1 O_3 concentrations may not be a fair representation of true surface concentrations so we have chosen to exclude the nighttime hours from the surface O_3 evaluation until the model's diagnostic layer 0 is complete.

The values used in the histogram were normalized to represent the fraction of observations at each monitoring station that fell within a given concentration range for the daylight hours over the model simulation period. For example, for station DRB (Derby, CT) there were 441 valid daylight observations covering the period July 14 - August 30, 1980 of which 15% fell in the range 5–20 ppb, 30% were in the range 5–40 ppb, 38% in the 40–80 ppb range, and 32% were >80 ppb. Similar data were compiled for the 214 monitoring sites and were then subjected to a cluster analysis to form coherent groups of sites based on frequencies of observed O_3 concentrations. The cluster analysis procedure used here performs disjoint clustering on the basis of minimizing the sum of squared distances from cluster means (SAS, 1982). Six groups of sites were formed using this analysis. Table 5.2 summarizes the histogram data for each group showing the mean and standard deviation

¹Concentrations of O_3 less than 5 ppb were not used in this analysis because they are within the noise limits of most monitors.

TABLE 5.2. MEAN AND STANDARD DEVIATION OF NORMALIZED FREQUENCY DISTRIBUTION OF DAYLIGHT (0800 - 1900 h, LST) OBSERVED O₃ CONCENTRATIONS AT MONITORING SITES IN SIX GROUPINGS.

	Ozone Concentration Range (ppb)			
	5-20	5-40	40-80	> 80
GROUP 1 (35 SITES)	.084 (.043)	.271 (.063)	.385 (.045)	.344 (.056)
GROUP 2 (39 SITES)	.149 (.058)	.378 (.067)	.406 (.072)	.216 (.033)
GROUP 3 (64 SITES)	.159 (.061)	.438 (.068)	.466 (.073)	.096 (.046)
GROUP 4 (54 SITES)	.218 (.063)	.590 (.060)	.355 (.043)	.054 (.040)
GROUP 5 (20 SITES)	.423 (.133)	.799 (.093)	.187 (.081)	.014 (.024)
GROUP 6 (2 SITES)	.044 -	.262 -	.627 -	.111 -

of the normalized frequency data in each concentration range. Full listings of the histogram data for each site by group are provided in Appendix C. Also, Figure 5.2 shows the locations, by ROM grid cell, of the sites included in each of the groups.

The monitoring sites in groups 1 and 2 generally observed the highest frequency of O_3 concentrations greater than 80 ppb. The stations in each of these groups tend to be located along the Northeast Corridor as shown in Figure 5.2. Lower O_3 levels were characteristic of groups 3 and 4. Nearly half the values in group 3 fell in the 40–80 ppb range, while over half of the group 4 values were within the tropospheric background value range for O_3 . These sites also tend to be geographically discriminated. The sites in groups 3 and 4 are more widely distributed across the Northeast than those in groups 1 and 2. Those in group 3 are predominantly in the southern and southwestern portion of the ROM domain and those in group 4 are more generally in the northern tier of states and Canada.

The sites in group 5 contain anomalously high frequencies of concentrations less than 40 ppb over half of which are actually less than 20 ppb. This is a highly uncharacteristic profile for daylight O_3 values and indicates that either the site was affected by a nearby NO_x source much of the time or that the monitor itself was out of calibration or had other problems. The sites in group 6 show relatively few values at either end of the distribution with the great majority of values in the moderate O_3 range. This distribution is characteristic of very rural or remotely located monitoring sites. Ideally, for regional model evaluation we would like a large number of these type sites because they tend to be representative of large areas. However, in this analysis, only two such sites have been identified in this group. They are Whiteface Mountain in northern New York State and Long Point Park in southern Canada. These locations are considerably distant from local source influences. This analysis points to the need for additional remotely located O_3 monitors in the Northeast U.S. and southern Ontario.

5.1.3 Observed Data Filter

The spatial resolution of the ROM grid generates an inherent limitation on the ability of the model to resolve gradients in the predicted concentration data. The grid cell size, Δx , used in the Northeast U.S. application, nominally 18.5 km, dictates that the critical wavelength below which the ROM cannot resolve gradients in the concentration data is $2\Delta x$, or approximately 37 km. It is therefore appropriate to remove those high frequency components of the observed concentration data set corresponding to wavelengths below 37 km.

The observed concentration data are in the form of time series with hourly entries at each monitoring station. Since we are interested in filtering the high frequencies in the data in space coordinates we must transform the concentration

time series to concentration space series for each station. We use the wind speed occurring in the same grid cell as the O_3 monitoring station and for the same hour as the O_3 observation to map the time series to a space series. The space series of concentrations can now be applied to a high frequency filter.

The filter used here is Spencer's 15-pt smoothing function. Based on the particular frequencies we are attempting to eliminate and the transfer function corresponding to Spencer's filter, the space series of concentrations is linearly interpolated to regular 7.5 km intervals and then the smoothing function is applied. After smoothing, the space series is then mapped back to time coordinates again using the wind speed to perform the transformation. An example of the effect of the filter is shown in Figure 5.3. Here, the time series of O_3 at the FX1 (Fairfax, VA) monitoring site is plotted for the period of interest, July 13-August 31, 1980. The dashed line and crosses correspond to the original unfiltered data set and the solid line corresponds to the filtered data set. It is immediately obvious that the filter's impact is rather small on the time series as a whole. Rapid fluctuations in concentration peaks and valleys have been smoothed by the filter, but generally no concentration has been altered by more than a few ppb. This is not an unexpected result for O_3 because the secondary nature of this pollutant is not conducive to the sharp concentration spikes that occasionally appear in the time series of a primary pollutant. The occasional gaps in the time series record correspond to missing data periods. The filter was applied to all hourly O_3 data in the observed surface data base for all sites. Nighttime data were included in the filtering process although they were not considered in the comparisons with predicted data.

5.1.4 Predicted Data

As discussed above, the ROM's surface diagnostic layer is not yet operational. When it becomes available it will calculate an average concentration and a variance based on the heterogeneous emissions distribution within the surface grid cell. For now we are using the hourly averaged model predictions of O_3 in the lowest prognostic layer, layer 1, to compare with the observed monitoring data. Layer 1 is typically 100 to 500 m deep, with the greater depths occurring at night when the radiation inversion forms. Under well mixed conditions during the day, layer 1 is 100-300 m deep and comes fairly close to representing a surface prediction. We restrict our comparison of model predictions and observations to the daytime hours of 0800-1900, LST when convective mixing is greatest and the ROM's layer 1 well-represents the thermally mixed conditions near the surface. The highest O_3 concentrations typically occur in this period as well.

Model predictions were interpolated to the exact locations of the 214 monitoring sites using a biquintic polynomial scheme. These data were then used in

the statistical analysis of the 6 groups of aggregated station data. These analyses therefore were based on comparisons of the filtered observed and spatially interpolated predicted data within each of the groups discussed above. In addition to the group analyses, evaluation of the ROM's ability to replicate "plumes" of O_3 on the regional scale was tested by analyzing spatial patterns in the observed and predicted data. Here, the filtered observed and the hourly averaged grid predictions were used.

5.2 RESULTS

In this section we examine the ROM's performance at predicting surface O_3 concentrations from a number of perspectives. First, from the aggregated station groupings, the hourly concentrations are examined as concentration frequency distributions in the observed, and separately, in the predicted data sets. Next, again in the aggregated groups, analyses for daily maximum and 7-hr daylight O_3 concentrations are performed. These analyses make use of time series and other graphical comparisons in which there is a greater degree of pairing between observed and predicted concentration sets than was used in the previous analysis. Finally, spatial patterns of episode-maximum concentrations are qualitatively compared within a subdomain including the Northeast Corridor.

5.2.1 Grouped Station Analysis

The purpose of the statistical comparison of model predictions and observations of O_3 concentrations by station groupings, as discussed previously, is to verify whether the ROM is generating similar frequency distributions of concentrations compared to the observations over the full period of simulation and over groups of stations exhibiting similar distributions of observed O_3 . Significant variations in these distributions would imply that the model is missing some basic features that control the generation or transport of O_3 . Comparison of maximum O_3 values between observations and predictions is also necessary because of their importance in air quality analyses. The maximum value analysis, however, must be put in context by first studying the full frequency distribution of concentrations.

Figure 5.4 shows a comparison of the histograms of daylight O_3 concentrations for the 6 station groups and Table 5.3 presents a summary of the normalized frequency data. The results indicate that the ROM performs better at predicting O_3 concentrations greater than 40 ppb than it does at lower concentrations. Concentrations of 40 ppb and less were observed at the 6 groups of receptors from a high of 80% of the time (group 5) to a low of 26% of the time (group 6). The corresponding figures for predicted concentrations are 18% of the time (group 5) and 4% of the

TABLE 5.3. FREQUENCY DISTRIBUTION OF DAYLIGHT OBSERVED AND
PREDICTED O₃ CONCENTRATIONS WITHIN RECEPTOR GROUPS FOR THE PERIOD
14 JULY - 31 AUGUST 1980.

Percent of daylight (08-19 h, LST) O ₃ concentrations between:									
Group	Number of Sites	5 - 20 ppb		21 - 40 ppb		41 - 80 ppb		> 80 ppb	
		Obs	Pred	Obs	Pred	Obs	Pred	Obs	Pred
1	35	8	1	19	7	39	66	34	26
2	39	15	1	23	9	41	69	21	21
3	64	16	1	28	9	46	79	10	11
4	54	22	1	37	12	36	80	5	7
5	20	42	2	38	16	19	73	1	9
6	2	0	0	26	4	63	93	11	3

time (group 6). The histograms in Figure 5.4 clearly illustrate this disparity with the obvious bulge in the predicted distributions at moderate O_3 values in the 40–80 ppb range and the broader distribution of lower values in the observations.

The model's performance for predicting concentrations >80 ppb appears quite good from the data in Table 5.3, with the possible exceptions of groups 5 and 6. As discussed previously, the members of group 5 were selected based on their anomalously low O_3 concentration profiles. The possible reasons for these low values include effects the ROM cannot take into account; thus these sites should be biased low in comparison to the model's expected predictions. The data in Table 5.3 appear to confirm the expectation. Group 6 contains only 2 sites whose observed concentration distribution conforms to a pattern characteristic of remotely-located sites. The results for this group show the ROM to underpredict the occurrence of >80 ppb O_3 . Small errors in the flow field can cause significant errors in the predicted trajectories of air parcels from particular source areas. These errors tend to worsen with increasing distance from the source. Since the remote sites are located at larger distances from source areas, one possible reason for the ROM's underprediction of higher concentrations at these sites is errors in the trajectories of air parcels affecting the sites from major source areas (see discussion of determinism in regional air quality models in a previous section).

The results presented in the histograms and the data of Table 5.3 also show that the ROM predicts the occurrence of low-production O_3 levels (40–80 ppb) considerably more frequently (66–93% of the time) than do the observations (19–63% of the time). This result follows from the model's underestimation of the frequency of low O_3 levels and is probably related to the local source influence at many of the urban-oriented monitoring stations.

Figure 5.5(a-f) presents plots of the observed cumulative frequency distribution of daytime O_3 concentrations versus the predicted distribution for each of the 6 receptor groups. The solid line in each figure represents the line of perfect agreement between the distributions and the dotted lines show the $\pm 10\%$ error bounds about the solid line. Each '+' symbol represents a percentile level in the frequency distribution, and the decile levels from 10% to 100% are marked by the integers 1, 2, ..., 9, 0. For example, in group 1, approximately 80% of the observed O_3 concentrations and 90% of the predicted concentrations are less than 100 ppb.

The plots confirm the model's tendency to overpredict at lower concentration values over all groups. Group 1 contains the sites with the highest observed concentration values and the ROM shows a tendency of increasing underprediction with concentration level. The agreement between predictions and observations is best for groups 2–4 for moderate to high O_3 values, up through the 99.5% level of the frequency distributions. The maximum value of the distribution is consistently underpredicted by the model. Figure 5.5(e) confirms group 5's anomalously low ob-

servations by showing systematic model overpredictions. Most groups show a more horizontal tendency in the distribution below about the 70–80% level, indicating that the range of the model predictions at lower concentrations is narrower than that of the observations.

The apparent narrow range of O_3 concentration predictions from the ROM may be understood from the model's physical and chemical processes. For locations of the domain not under the influence of precursor emissions from significant sources or affected by transport of relatively high concentrations, the factors controlling the predicted O_3 concentration include the influence of specified boundary conditions and the inherent reactivity of the background atmosphere. Boundary conditions specified for this simulation were time-dependent and varied between 40 and 70 ppb at the upwind lateral boundaries and were fixed at 35 ppb at the top boundary of the ROM domain. The chemical mechanism used in the model, the Carbon Bond IV, contains a reaction accounting for the background reactivity of the atmosphere from the reaction of methane with the OH radical (Gery *et al.*, 1988). A constant methane concentration of 1.85 ppm is assumed. This reaction produces HO_2 radicals and formaldehyde which contribute to increased O_3 production. Thus the chemical mechanism itself contains a "built-in" potential to form background O_3 from natural sources.

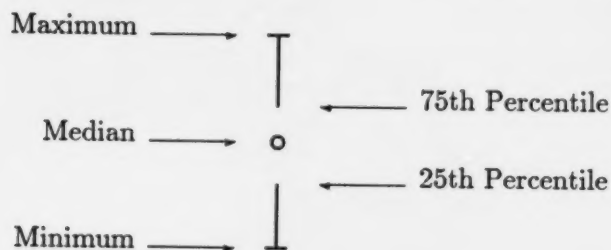
The two stations of group 6 in the simulation results demonstrate this background effect. The frequency distribution for this group shows that half of all daytime predictions were within the range of 35–50 ppb and that 80% of the predictions fell between 35 and 65 ppb. These sites are considerably distant from major sources and apparently were not frequently affected by transport of plumes from upwind locations. Their concentration distributions therefore reflect the boundary and background effects on O_3 . The observed distribution of O_3 at low concentrations for group 6 spans a broader range perhaps indicating more local influences or a lower background concentration than the model generated.

5.2.2 Grouped Station Analysis - Maxima and Block Averages

The primary ambient air quality standard for O_3 is designed to protect human health and focuses on the maximum one-hour daily concentration value. Although this value represents the extreme in the frequency distribution and, as such, is a difficult target to aim for in air quality simulation exercises, the ROM must perform credibly at predicting maximum values to be useful in analyses relating to the primary O_3 standard. A secondary O_3 standard is currently under discussion as a means of protecting welfare, including the nation's crop and forest lands, from pollutant damage. A secondary standard would most likely take the form of a longer time average than the single hour primary standard. As an example, we examine

the daily 7-hr average of O_3 concentrations from 0900 through 1600 h, LST as being representative of the type of statistic that may be used for secondary O_3 standard analyses. Most recently, consideration is being given to a longer term (8-hr) and shorter term (1-hr) primary and secondary O_3 standard by the EPA.

Figure 5.6 presents a time series of maximum concentrations from three of the station groups for the entire simulation period. For each day, maximum observed concentration values are plotted adjacent to maximum predicted values for the same station group. The concentrations are indicated as frequency distributions, showing the median value of the O_3 maxima from all members of the station group on any one day as the middle symbol. Maximum and minimum values of the O_3 maxima in the group are indicated by the outer ends of the bars bracketing the symbol, and the 25th and 75th percentiles are shown by the inner ends of the bars:



Station group 1, shown in Figure 5.6(a), indicates that the median values of the observed and predicted concentrations track quite well through the simulation period. Generally, the observed median is somewhat greater than the predicted median during periods of higher concentration. At the 75th percentile the ROM tracks the observed temporal trend, although the concentrations are underpredicted during most episodes. The maximum in the distribution also is typically underpredicted, particularly during episodes. Some episodic periods seem to be handled better than others by the model. For example, the concentrations during the episodes of Julian days 196-199, 207-209, and 238-241 show good agreement between observations and predictions while the ROM did not perform as well for the episodes of 201-203 and 212-215. The spatial pattern analysis of concentration fields shown later should help determine whether plume misalignment is a cause of the poorer comparison during some episodes. The minimum concentration in the distribution of maxima is usually greater in the predictions and the entire range of maximum concentrations seen among the stations in group 1 is almost always smaller in the predictions than the observations. This is consistent with the previous analysis of all concentration data and the fact that subgrid scale processes can cause local fluctuations in the observed O_3 concentration data that are greater than the ROM can predict. This would be especially true for maximum values, which are outliers in the frequency

distribution.

The time series for group 3 is shown in Figure 5.6(b). The frequency of concentrations of > 80 ppb O_3 in this group is lower than in group 1 and the stations are more geographically distributed in the ROM domain compared to the stations in group 1 which are almost exclusively in the Northeast corridor. The figure shows that the temporal trends in the model results are again comparable to those in the data. The occurrence of underprediction of the median value in the distribution is less frequent than in group 1 and the maximum value is even occasionally overpredicted. For group 6, the remote stations, the time series of average daily maxima is plotted since there are only two sites in the group. The temporal trend in the ROM results follows the observed trend fairly well although the predicted maxima are generally lower than the observed. The placement of predicted plumes is critical in this group because of the small number of stations. For example, the ROM picked up the influence of the day 196–198 episode on the remote sites but did not show as much influence for the day 201–204 episode as was noted in the observations. In general, for group 6, the ROM underpredicts the higher O_3 values but matches the observations on days with lower values when observed concentrations are more likely influenced by regional formation and transport rather than long range transport of individual plumes.

The median values from the daily data set presented, in part, in Figure 5.6 were aggregated for analysis. The results for station groups 1 through 5 are shown in Figure 5.7. The symbols represent the mean value of the daily medians through the simulation period and they are bracketed by the 95% confidence interval about the mean. The figure shows the decrease in maximum O_3 concentration from group 1 through group 5 in the observations as well as the predictions, although the gradient is greater in the observations. The median is slightly underpredicted in group 1 and is overpredicted in the remaining groups. Since the confidence intervals of the predictions and observations overlap in groups 1 through 3 the median values are essentially the same while for groups 4 and 5 the overprediction is significant. The overprediction in group 5 is expected because of the anomalous nature of the members of the group as previously discussed. These data are also presented in Table 5.4.

Another perspective of the model performance can be gained by analyzing the bias in the predictions of maximum O_3 concentrations. The bias, or residual concentration, is defined as:

$$Bias = O_{3,Obs}^{Max} - O_{3,Pred}^{Max}.$$

For each station group the bias was calculated for each member of the group for each day of the simulation period. In this way the observed and predicted O_3 maxima for a given day were matched in space but not in time. The bias values were then sorted into fixed ranges according to the associated value of $O_{3,Obs}^{Max}$. For example,

TABLE 5.4. STATISTICS OF THE DAILY MEDIAN OF MAXIMUM HOURLY O₃ CONCENTRATIONS (OBSERVED AND PREDICTED) AT ALL SITES IN STATION GROUPS 1-5 OVER THE SIMULATION PERIOD 80196 - 80243

		Ozone Concentration (ppb)				
		Mean	± 95% Confidence Interval	Std. Dev.	Minimum	Maximum
GROUP 1	Obs:	88.1	7.8	27.3	37	138
	Pred:	82.6	4.8	16.8	54	122
GROUP 2	Obs:	76.9	7.1	24.7	27	122
	Pred:	79.5	4.4	15.4	53	112
GROUP 3	Obs:	64.5	4.6	16.0	30	92
	Pred:	70.1	2.6	9.1	54	92
GROUP 4	Obs:	54.4	4.3	14.9	24	91
	Pred:	65.1	2.1	7.4	50	86
GROUP 5	Obs:	39.8	3.5	12.1	21	75
	Pred:	66.0	2.4	8.5	50	86

all bias values associated with maximum observed concentrations between 60 and 80 ppb would fall into one range. The bias values for maximum O_3 are plotted in Figure 5.8 as a function of observed O_3 value in discrete 20 ppb ranges. The bias value shown for each range is the mean and the 95% confidence interval about the mean is indicated. The number of bias values occurring in each range is shown toward the bottom of the figure.

Figure 5.8 shows a clear systematic trend of increasing underprediction of maximum O_3 with increasing concentration. This trend occurs in all station groups. The data show that O_3 maxima are generally overpredicted for observed maximum values less than 80 ppb and are underpredicted for values above 80 ppb. The ROM performs best for maximum O_3 concentrations of 60–100 ppb. The trends in these bias plots can be understood from the previous analyses showing the range in the observed data to be greater than the concentration range in the predicted data. As one moves farther from the part of the distribution where the agreement is best, the absolute bias can be expected to increase because of the differing nature of the distribution in observed and predicted values. Figure 5.8 shows some evidence that for the highest concentrations, perhaps over 140 ppb, the model's underprediction levels off, especially for groups 3 and 4. These values are likely associated with major source plumes in significant episodes and, provided the flow fields are reasonably accurate, the ROM should handle these cases well. The number of cases of maximum O_3 between 100 and 140 ppb is significantly greater than those over 140 ppb and probably represent a wider range of meteorological conditions and flow fields. The ROM shows a wider variation in performance at these levels than for the higher levels. In general, Figure 5.8 shows that the mean underprediction of maximum O_3 concentrations is ≈ 30 ppb for observed values of 120–140 ppb, increasing to 50–70 ppb for observed values >160 ppb.

Table 5.5 presents a summary of statistics on the average of the median values of maximum O_3 in this data set as well as the average of the median bias of maximum O_3 values. The normalized bias is also shown. Note that this data set has been constructed in a different manner than the one summarized in Table 5.4. Here the median values of maximum O_3 concentrations were chosen for each station separately for the full simulation period. In Table 5.4 the medians were chosen for each day separately from among all stations. The data in Table 5.5 show that the ROM slightly underpredicts the median concentration for groups 1 and 6 (3.8% and 6.3%, respectively), and overpredicts in the other groups. Values of the absolute normalized bias for all groups except group 5 are less than 25%. Appendix D contains listings of the full data set for each station group, including maximum observed and predicted O_3 concentrations and bias.

Next, the 7-hr block average (0900–1600 h, LST) of O_3 concentrations is analyzed for the station groups. This time average has been discussed as one possible measure for assessing the effects of air quality for a secondary O_3 standard. The

TABLE 5.5. SUMMARY OF STATISTICS ON MEDIAN OF STATION MAXIMUM O₃ VALUES

	(A) O ₃ , Max (Obs.) ppb	(B) O ₃ , Max (Pred.) ppb	(C) O ₃ , Max (Obs.)-O ₃ , Max (Pred.) ppb	$\frac{C}{A} \times 100$
GROUP 1	87.6	79.8	+ 3.4	+ 3.8%
GROUP 2	73.8	76.7	- 4.8	- 6.5%
GROUP 3	62.5	69.0	- 7.8	- 12.5%
GROUP 4	52.4	64.2	- 11.7	- 22.3%
GROUP 5	36.6	62.2	- 25.5	- 69.7%
GROUP 6	72.0	66.0	+ 4.50	+ 6.3%

time series of 7-hr averages for groups 1, 3 and 6 are shown in Figure 5.9. The observed and predicted data are again shown as frequency distributions of all data for one day among all stations in the group. The trends shown in Figure 5.9(a) for group 1 are generally similar to those shown for the daily maximum concentrations, although the magnitudes of the 7-hr average are less than the daily maxima and the range of the concentration distribution is narrower for the 7-hr average. The ROM predictions track the observed data fairly well here. The temporal gradients in the concentrations are smaller in the predictions than the observations. For group 3, shown in Figure 5.9(b), the median values in the time series are consistently overpredicted, similar to the results shown for the daily maxima in group 3, although the effect appears to be more systematic for the 7-hr averages. The maxima in the distributions for group 3 show both underpredictions and overpredictions, while the minima are consistently overpredicted.

The time series of 7-hr averages for group 6 is shown in Figure 5.9(c). The observed and predicted data show corresponding patterns. When the observed data show relatively higher concentrations the predictions are also high, but somewhat below the levels of the observed. During the middle part of the simulation period when the predicted data indicated a consistent 50–60 ppb daytime background concentration, the observations showed more day to day variability ranging from 40–70 ppb. The episode of Julian days 239–240 was picked up in the simulation results, although the observations showed an end to the episode and a rapid drop in the O_3 concentrations on days 241 and 242 while the model showed continued elevated concentrations. The trajectories of individual plumes, as discussed previously, can have a more pronounced effect on the results for group 6 than for the other groups because of the small number of stations.

Table 5.6 presents a summary of statistics on the daily median of the 7-hr averages shown in Figure 5.9. These data are analogous to those presented in Table 5.4 for maximum O_3 concentrations. The confidence intervals about the mean for the observed and predicted values in group 1 overlap, indicating no significant difference between the mean values. In the other groups the ROM consistently overpredicts the mean value by an increasing margin as the mean observed concentration decreases. These data are also presented in Figure 5.10. The maximum values of the 7-hr average are predicted more accurately than the means. The picture that emerges from the data of Tables 5.4 and 5.6 is that the ROM performs better at predicting both maximum O_3 concentrations and 7-hr average concentrations when these values are consistently above background levels and especially when values above ≈ 60 ppb are observed.

Figure 5.11 presents bias values and their 95% confidence intervals as a function of observed concentration for the 7-hr O_3 averages. These data were calculated in a similar manner to the data presented for the maximum O_3 data set shown in Figure 5.8. The trends in model performance seen for the maximum O_3 concentra-

TABLE 5.6. STATISTICS OF THE DAILY MEDIAN OF 7-HR AVERAGE O₃ CONCENTRATIONS (OBSERVED AND PREDICTED) AT ALL SITES IN STATION GROUPS 1-5 OVER THE SIMULATION PERIOD 80196 - 80243

		Ozone Concentration (ppb)				
		Mean	± 95% Confidence Interval	Std. Dev.	Minimum	Maximum
GROUP 1	Obs:	64.4	5.9	20.7	28.9	100.5
	Pred:	67.3	3.7	13.0	42.0	90.9
GROUP 2	Obs:	54.3	5.3	18.7	22.1	86.4
	Pred:	64.7	3.4	12.0	42.7	92.9
GROUP 3	Obs:	45.7	3.7	12.9	22.6	68.2
	Pred:	58.3	2.2	7.6	42.0	71.4
GROUP 4	Obs:	37.8	2.9	10.3	19.2	62.9
	Pred:	54.7	1.7	5.9	43.9	67.0
GROUP 5	Obs:	25.6	2.5	8.6	13.4	50.6
	Pred:	54.0	2.3	8.0	35.9	70.4

tions are again demonstrated in Figure 5.11. The model performance is best in all groups for observed concentrations of 60–100 ppb with increasing underprediction for concentrations above this range and increasing overprediction for concentrations below this range. There are relatively few 7-hr average observed O_3 concentrations above 120 ppb during the simulation period; thus, the significance of the trend at higher concentrations is not as great as that for the maximum O_3 analysis.

Table 5.7 presents a summary of statistics on the average of the median values of 7-hr average O_3 in this data set along with the average of the median bias of 7-hr average values and the normalized bias. The corresponding data set for maximum O_3 values was shown in Table 5.5. The absolute normalized bias values for the 7-hr averages are generally greater than they are for the maximum O_3 concentration bias values. In this analysis, groups 1, 2, and 6 have normalized biases less than 25%, while in the maximum O_3 concentration analysis the bias of all groups but one were within 25%. Groups 3 through 6 show average values of the 7-hr prediction between 50 and 57 ppb, within the range of the expected daytime background value in the simulation. The average observed values, however, drop as low as 23 ppb leading to increasing overprediction with decreasing concentration below 50 ppb. Appendix E contains listings of the full data set for each station group for the 7-hr average O_3 concentrations.

Similar analyses were performed for station group data for the 11-hr block average from 0800–1900 h, LST. Results from this analysis are not presented here however, because of their similarity to the 7-hr average results.

5.2.3 Spatial Pattern Analysis

In addition to the grouped station analyses discussed above, the ROM results for O_3 were analyzed for agreement in spatial patterns between the predictions and the observations. For the spatial analysis, we have considered a subregion of the full ROM domain, shown in Figure 5.12, containing the urban areas of the Northeast Corridor. The purpose of the spatial analysis is to indicate whether there are potential problems in the location and extent of O_3 “plumes” from major precursor source areas. Misalignment of these plumes can produce a poor statistical comparison between paired predicted and observed concentrations when the simulated plume may be only slightly translated from its true position.

Five episodes of relatively high O_3 levels from within the entire simulation period are studied here. The analysis considers the contoured pattern of maximum hourly O_3 concentrations for the entire episode. Predicted concentrations are determined for each individual ROM layer 1 grid cell and then objectively contoured with computational techniques. Observed concentrations were taken from all available monitoring sites using the filtered data set described earlier. Since many of the

TABLE 5.7. SUMMARY OF STATISTICS ON MEDIAN OF STATION 7-HR. AVERAGE O₃ VALUES

	(A) O ₃ , 7-hr. (Obs.) ppb	(B) O ₃ , 7-hr (Pred.) ppb	(C) O ₃ , 7-hr. (Obs.)-O ₃ , 7-hr (Pred.) ppb	$\frac{C}{A} \times 100$
GROUP 1	63.7	65.8	- 4.7	- 7.4%
GROUP 2	51.4	62.3	-12.0	- 23.3%
GROUP 3	43.9	56.5	-13.6	- 31.0%
GROUP 4	35.8	53.9	-17.6	- 49.2%
GROUP 5	23.6	51.0	-27.1	-114.8%
GROUP 6	50.0	53.4	- 1.41	- 2.8%

monitoring sites are located in or very near urban areas, with the potential for local O_3 scavenging effects, the data can be highly variable and, therefore, do not lend themselves well to objective contouring. Subjective contours have been drawn by the authors for the observed data sets. In so doing, we have tried to maintain the integrity of the O_3 fields by ignoring obvious outliers and using discretion in placing contours so as not to oversmooth the data. Large areas of uncertainty still remain in the patterns of the observed concentrations, especially in data-sparse regions to the west of the Northeast Corridor and to the east over the ocean.

The patterns discussed below compare the results of the maximum hourly O_3 concentrations over the episode. These concentrations are determined for each ROM grid cell individually (predicted values) and for each monitoring site individually (observed values). The episodes considered here range from 3 to 10 days in duration. The analysis of the composite of maximum values over the episode follows from the quasi-deterministic use of ROM results. This use indicates that individual station values may be considered separately only when relatively long time periods are also used in the analysis. While patterns for individual days are not discussed here they are presented in Appendix F for the days composing the episodes considered. It is useful to examine these daily patterns to sense the variability that is inherent in the episode-composite patterns, although a direct comparison of daily patterns constitutes a deterministic analysis that is not advocated here.

Episode 1: 80196 - 80199 (July 14 - July 17, 1980)

This period was characterized by a large high pressure system over the mid-Atlantic states which slowly drifted to the southeast. Winds at the surface were generally from the south-southeast through southwest along the East coast, while winds aloft were westerly. Maximum surface temperatures reached the upper 90's to low 100's°F. The episode ended when a weak cold front moved across the area on July 17 bringing with it a new air mass.

The contours of maximum observed O_3 concentrations above 120 ppb for this episode are shown in Figure 5.13(a) and the contours of the predicted values are shown in Figure 5.13(b). The 120 ppb contour is darkened in the predicted map. (The 120 ppb cutoff has been chosen here because it is the current level of the NAAQS in federal air quality regulations.) The areas encompassed by +120 ppb O_3 values agree fairly well in observations and predictions. The observed values show a maximum O_3 area over south-central CT with concentrations in the range of 250-300 ppb. The predictions show a similarly aligned pattern of maximum O_3 from 180 to 200 ppb over eastern CT and RI, with another maximum area from 200-220 ppb over eastern Long Island. No monitoring stations exist in the eastern sections of Long Island. Another area of high predicted concentrations is in the Baltimore-Washington (BW) corridor with concentrations from 180-200 ppb. This agrees very closely with the observations in that area. The higher O_3 levels

observed downwind of Philadelphia over central NJ are essentially absent from the model predictions. The model shows an area of +160 ppb O₃ east of the central NJ coast over the ocean, but it is not clear whether this plume has originated from the Philadelphia source area.

Episode 2: 80202 - 80204 (July 20 - July 22, 1980)

A Bermuda high pressure system controlled the air flow during this 3-day period over the Northeast U.S. Winds at the surface and aloft were generally from the southwest. Maximum surface temperatures again were in the upper 90's to near 100°F. Some late afternoon thunderstorms occurred in the Northeast Corridor. A weak stationary front over the Great Lakes area eventually brought the episode to a close when the front moved closer to the Northeast bringing considerable cloudiness and rain showers in advance of a new air mass.

Figures 5.14(a) and 5.14(b) show the contours of the episode maximum hourly observed and predicted O₃ concentrations, respectively. The general patterns of concentrations agree quite well, especially those areas above 160 ppb in New England, where the simulated plume alignment appears to be in excellent agreement with concentrations. The highest predicted concentrations appear over central CT and eastern Long Island with concentrations from 180-200 ppb. The maximum observed concentrations appear in the same area, but with values generally from 200-250 ppb. The ROM has underpredicted maximum O₃ concentrations in the BW corridor and over central NJ. The effects of the Philadelphia area emissions on the O₃ patterns appear farther downwind than the observations would lead us to believe. There are, however, insufficient monitors in the central NJ coastal area to extend the analysis of the observed pattern. The ROM has underestimated the spatial coverage of +120 ppb O₃, especially in the southern portions of the Northeast Corridor.

Episode 3: 80207 - 80209 (July 25 - July 27, 1980)

This 3-day episode occurred under conditions of a stagnating high pressure system over the mid-Atlantic states. Winds near the surface were generally light and from a south through southwest direction. Aloft the winds were stronger and from the west at the beginning of the period turning to the southwest by the end. Maximum afternoon surface temperatures varied from the upper 80's to the low 90's°F. Showers associated with a stationary front just to the west of the Northeast Corridor ended the episode.

The maximum hourly O₃ concentrations observed during the episode are contoured in Figure 5.15(a). Concentrations over 120 ppb are shown to extend from the BW area northeastward into Massachusetts. Maximum observed concentrations between 150 and 170 ppb were observed over central and northeast NJ and over

western Long Island. Contours of maximum predicted concentrations, shown in Figure 5.15(b), map out spatial areas of +120 ppb O₃ that are aligned directionally with those of the observed concentrations, but shifted slightly to the south. The areas of highest predicted concentrations from 140–165 ppb over south central NJ and Long Island show very similar spatial coverage as the highest observed areas, but again they are shifted slightly in space. Interestingly, the model predictions downwind of Philadelphia for this episode show better agreement with observations than some of the other episodes.

Episode 4: 80212 - 80221 (July 30 - August 8, 1980)

The fourth episode was one of 10 days duration when a large Bermuda high pressure system over the western Atlantic built a ridge of high pressure over the eastern U.S. The meteorological system was quasi-stationary. A stationary front aligned east-west across the middle Atlantic states drifted north and south during the period. To the south of the frontal zone surface winds were light and from a south to southwest direction and maximum surface temperatures varied from the low to upper 90's°F. For those areas that were occasionally on the north side of the frontal zone the winds were from the northeast and the maximum surface temperatures varied from the mid 80's to near 90°F. Winds aloft were from the west and southwest during the period. An upper level high pressure ridge dominated the East coast. The weakening of this ridge and the subsequent cold frontal passage and air mass exchange ended the episode.

Figures 5.16(a) and (b) contain contours of maximum hourly O₃ concentrations over the 10 day period for the observed and predicted data sets, respectively. The areas of concentration over 120 ppb in the observations and the predictions roughly correspond, except for a gap in the predicted area from DE through northern and central NJ. The area of high O₃ concentrations from 140–200 ppb over central NJ downwind of Philadelphia has not been predicted well by the ROM. Areas of 140–180 ppb O₃ are predicted farther east, over the Atlantic. To the northeast, an area of +160 ppb O₃ concentrations is observed over CT and RI. The predicted pattern shows a large area of +160 ppb O₃ over the water, with part of the area covering CT and Long Island. Maximum model predictions (180–185 ppb) are lower than maximum observations (200–250 ppb) over this area. To the south, the effect of the BW corridor in the predicted concentration pattern is seen mostly on an east-west axis with maximum values in the 140–160 ppb range. The observations show an effect with a southwest-northeast axis with maximum concentrations from 160–180 ppb, although this directional bias may be a function of station locations in this area.

Episode 5: 80238 - 80241 (August 25 - August 28, 1980)

This four day episode was characterized by a stationary high pressure system centered over the mid-Atlantic states with an upper level ridge over Missouri. The upper level high pressure system weakened and moved to the Southeast coast during the second two days. The wind flow near the surface was light and disorganized with a predominant northeasterly component especially near the Atlantic coast. The flow aloft showed moderate northeasterly flow along the coast and more disorganized flow inland. As the episode progressed the flow aloft turned more consistently from the Northwest and the surface winds became southerly and southwesterly. Surface temperatures generally varied from the mid 80's to mid 90's°F. A cold frontal passage late on August 28 ended the episode.

Figures 5.17(a) and (b) present the contours of maximum hourly O_3 concentrations during this episode for the observations and the ROM predictions, respectively. It is interesting to note the 160 ppb contour in the observed O_3 field. It is somewhat "bowtie" shaped with bows at the southwest end over eastern PA and at the northeast end over CT and Long Island. There are pockets of near 200 ppb concentration through this envelope with a few +200 ppb values in CT and Long Island. From the individual day maps for this episode shown in Appendix F one sees an O_3 plume extending to the southeast over NJ and eastern PA during the first two days of the episode, corresponding to northeast flow, and in the second two days the plume is seen extending to the northeast over CT, corresponding to southwest flow. The flow reversal during the episode and the otherwise light wind speeds make this a particularly difficult episode to model well. Model predictions show large areas of +120 ppb O_3 over the region, corresponding roughly to those seen in the observations. There are underpredicted areas however, especially over CT and NJ. The ROM has modeled well the area of 120-140 ppb O_3 over southeast PA. The plume over the BW area is overpredicted in terms of its magnitude by about 20 ppb, but the location is accurately predicted. The ROM predicts a large area of 140-160 ppb O_3 over the ocean east of NJ; the shoreline monitors give some indication that this is a credible prediction.

These five episodes include essentially all of the significant regional high O_3 events that were observed in the Northeast during the simulation period. In examining the ROM's performance at predicting the maximum O_3 concentrations over these episodes a number of impressions are elicited. First, the model has produced O_3 plumes from all of the major metropolitan source areas along the East coast. The dimensions and magnitudes of these plumes are comparable to those seen in the observations. Plume placement tends to be shifted slightly clockwise over the ocean as compared to that seen in the observations. The monitoring stations are, of course, biased because they are all land-based, so we do not have an adequate picture of O_3 concentrations off-shore. The interpolated wind fields used to drive the trans-

port portion of the model may also have introduced some bias in the directional transport off-shore.

Several other deficiencies were also noted. The ROM's predictions downwind of the Philadelphia area tend to be low compared to observations. Only during one of the episodes studied (Episode 3) was the plume predicted well. In a number of cases the model predictions showed a maximum impact off the New Jersey coast. Both transport and emissions problems may be causing the errors here. Also, the ROM does not predict the very highest O₃ concentrations well in the plumes, especially downwind of the New York area. Monitored values of +225 ppb, as high as 300 ppb, are nearly all underpredicted. Typically these values are associated with large spatial gradients in the plume, and the ROM's grid resolution is a limiting factor in predicting these sharp peaks. Nevertheless, despite these problems, the model's ability to accurately define O₃ plumes on the regional scale appears good. It is important to view the spatial patterns from this broad perspective because small errors in plume location can produce large apparent errors in statistical comparison of data at individual station locations.

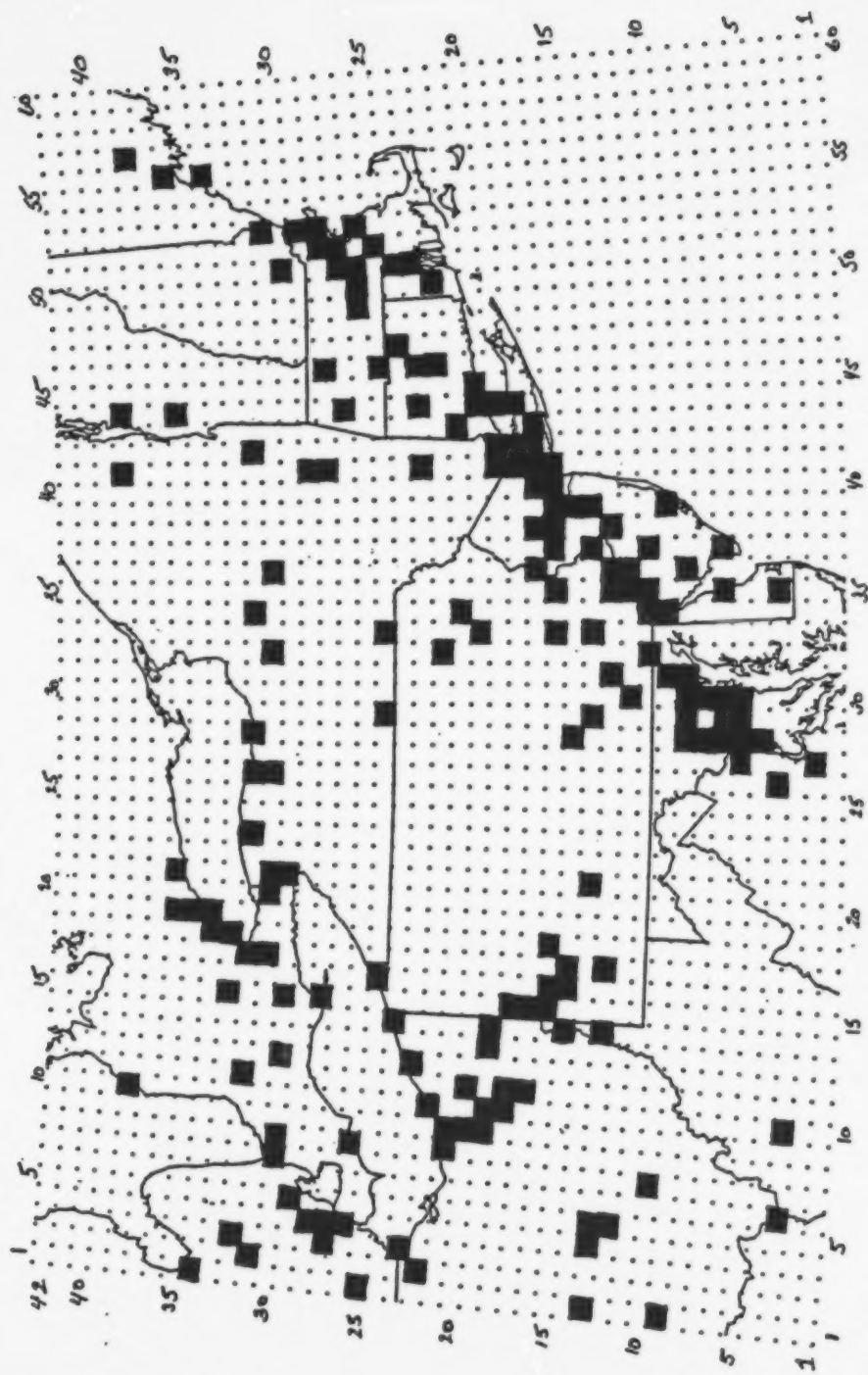
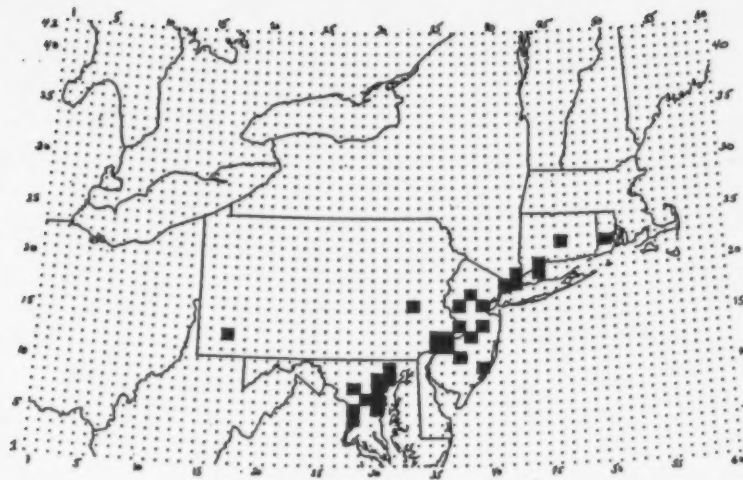


Figure 5.1. ROM grid cells (darkened) containing O₃ monitors.

GROUP 1



GROUP 2

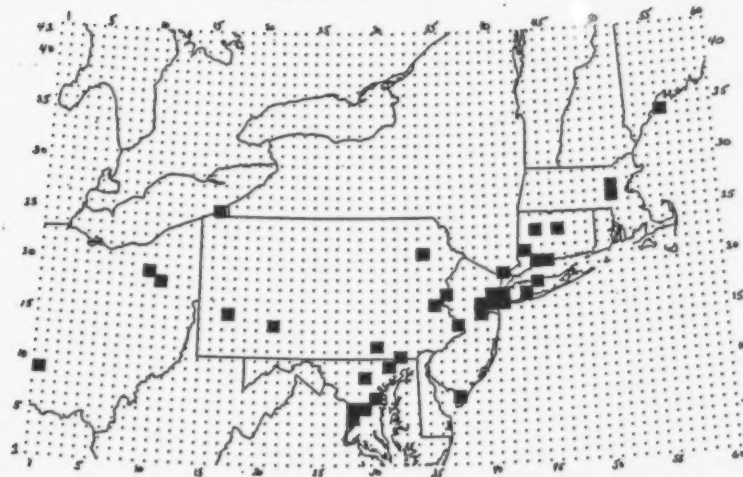
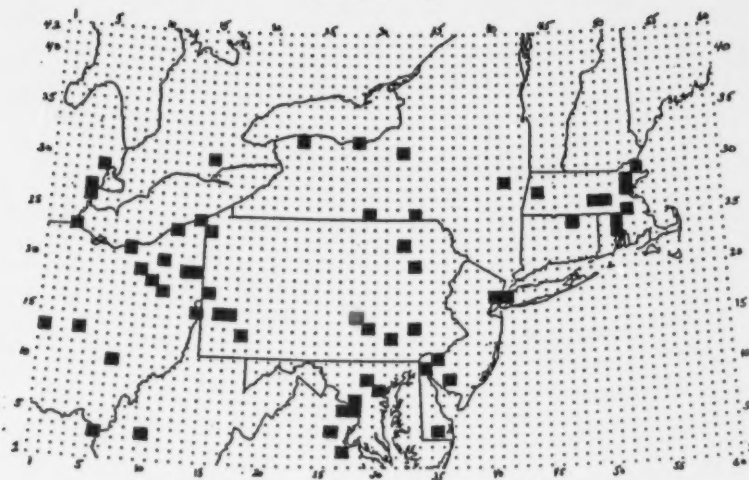


Figure 5.2. ROM grid cell locations (darkened) of monitoring sites within groups 1 through 6.

GROUP 3



GROUP 4

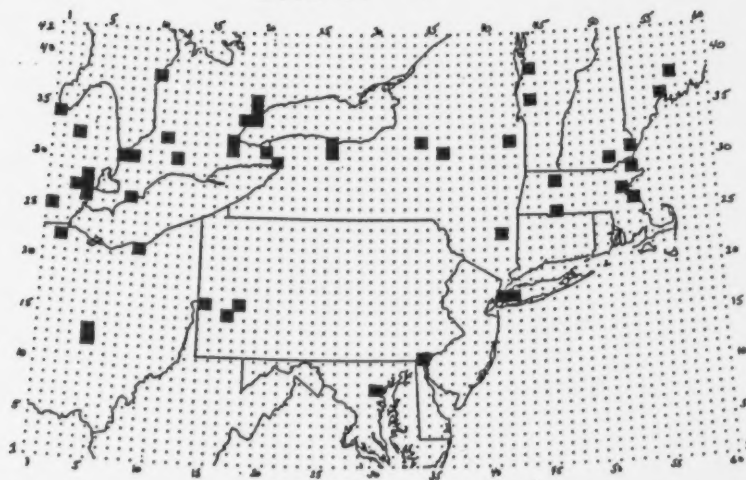
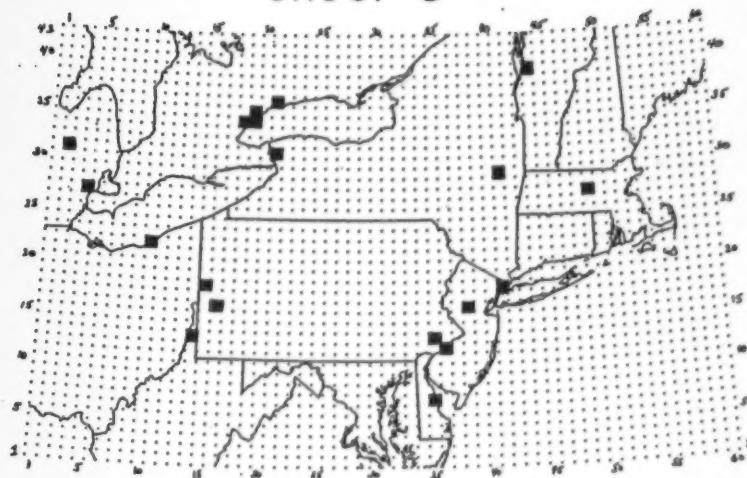


Figure 5.2. (continued)

GROUP 5



GROUP 6

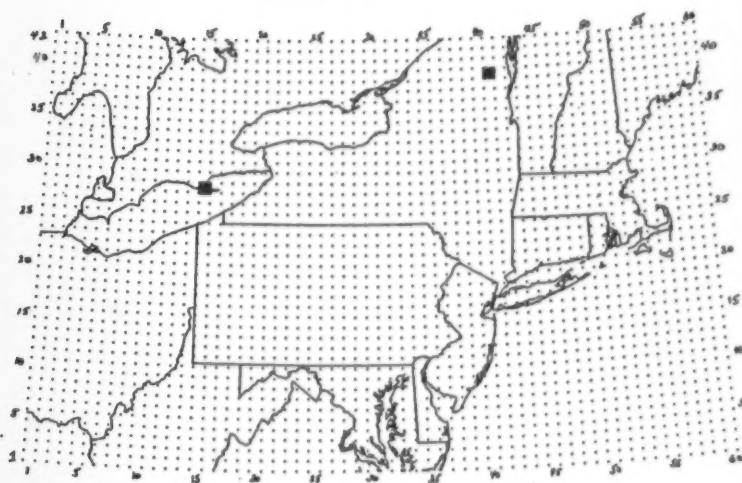
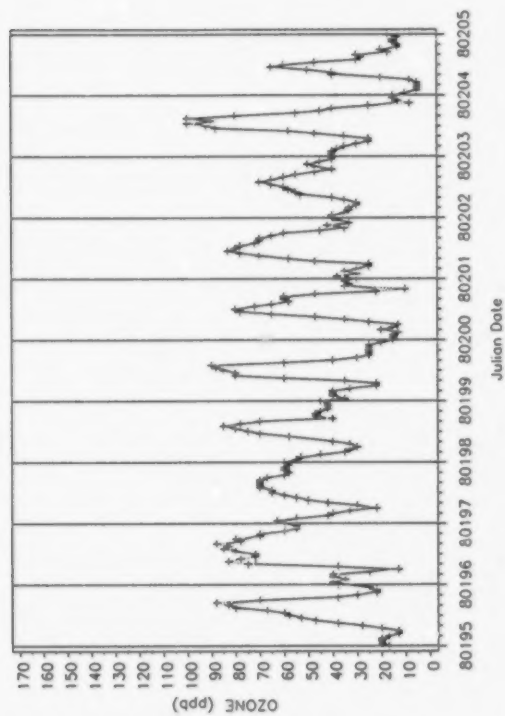


Figure 5.2. (continued)

FAIRFAX SITE: FX1 VA10400050



FAIRFAX SITE: FX1 VA10400050

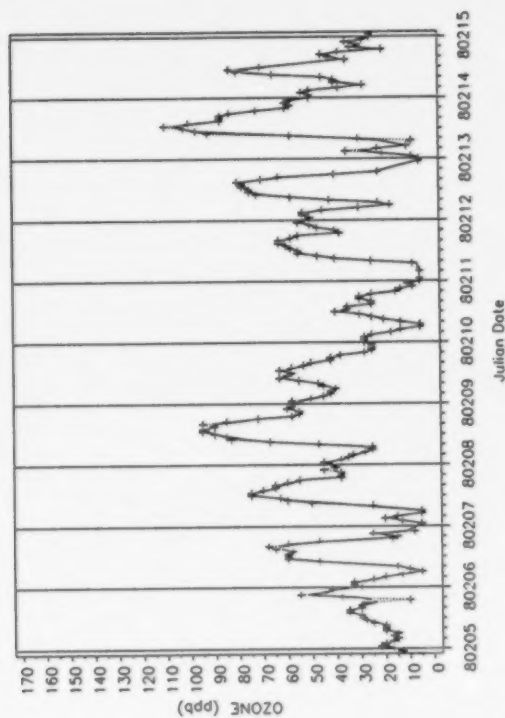
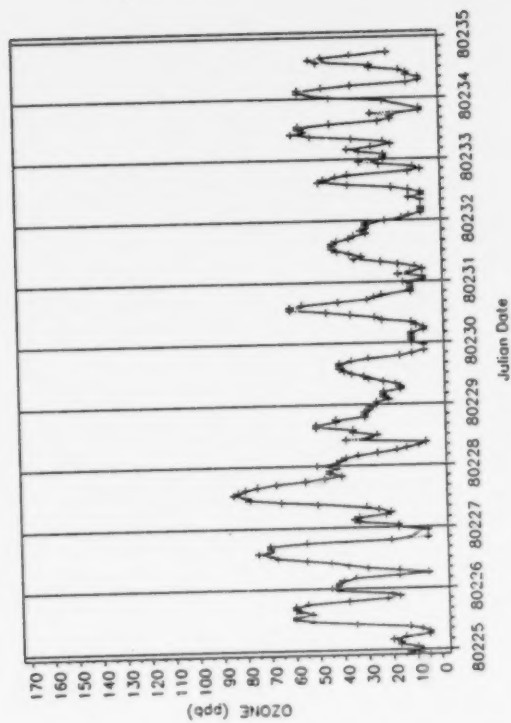
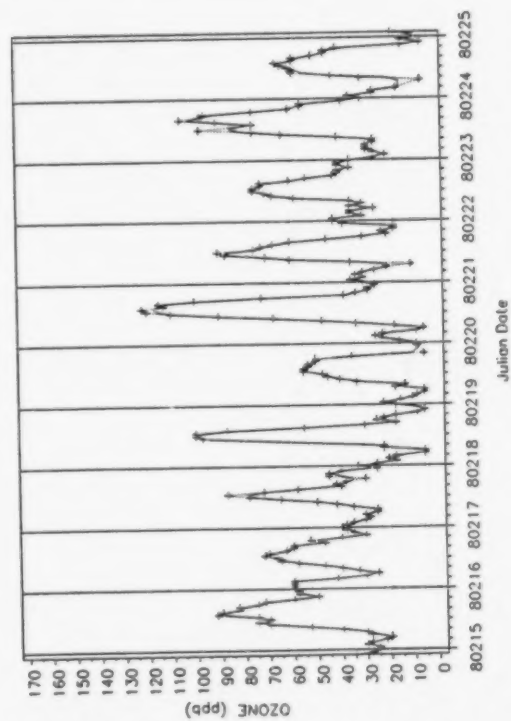


Figure 5.3. Time series, filtered and unfiltered, of FX1 observed O₃ data. The solid line is the filtered data set, and the dotted line is the unfiltered data set.

FAIRFAX SITE: FX1 VA10400050



FAIRFAX SITE: FX1 VA10400050



FAIRFAX SITE: FX1 VA10400050

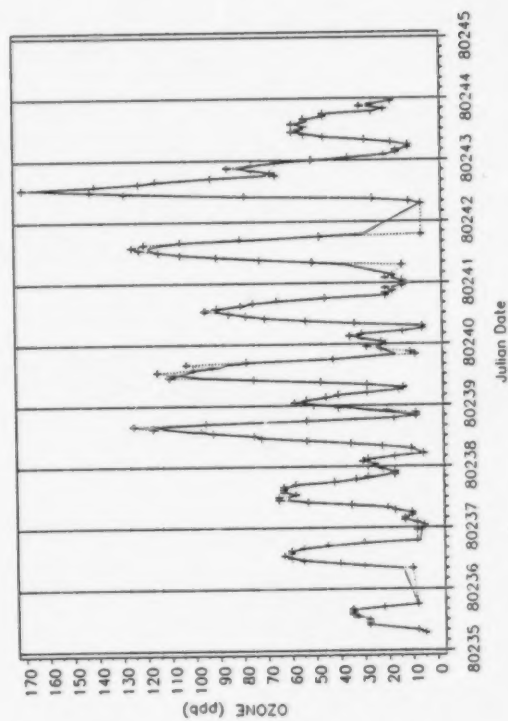
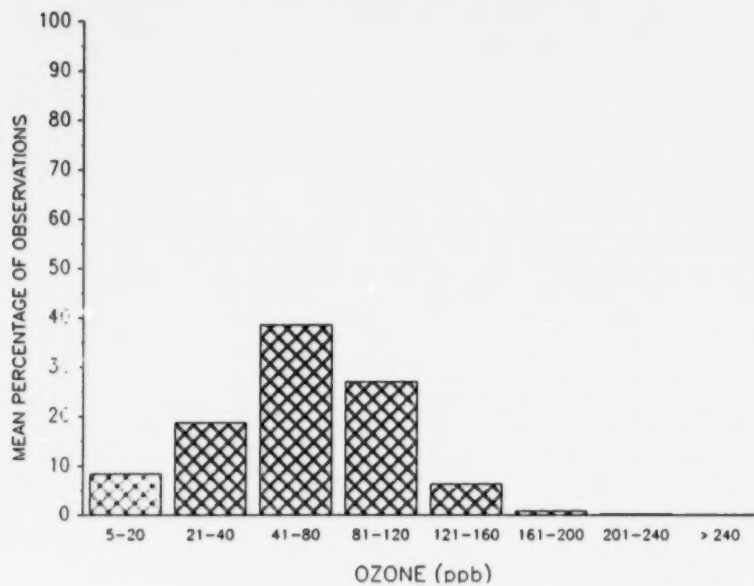


Figure 5.3. (continued)

SURFACE OZONE ANALYSIS

GROUP ONE OBSERVED (DAYLIGHT HOURS)



SURFACE OZONE ANALYSIS

GROUP ONE PREDICTED (DAYLIGHT HOURS)

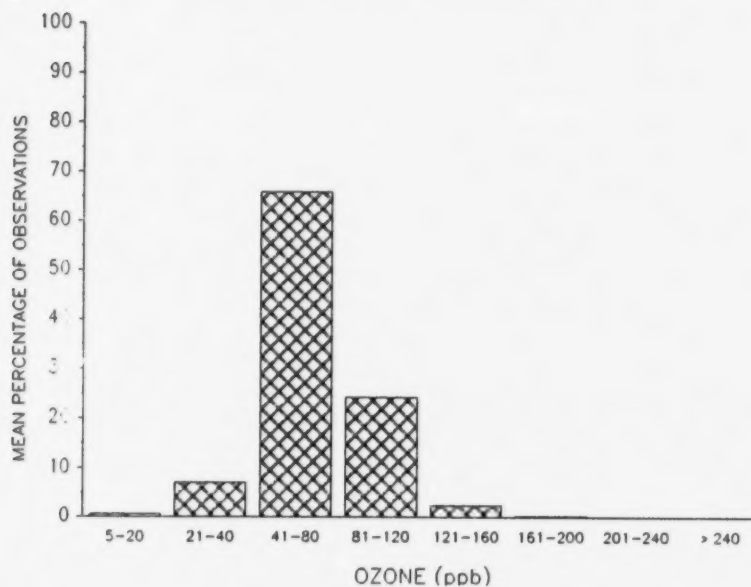
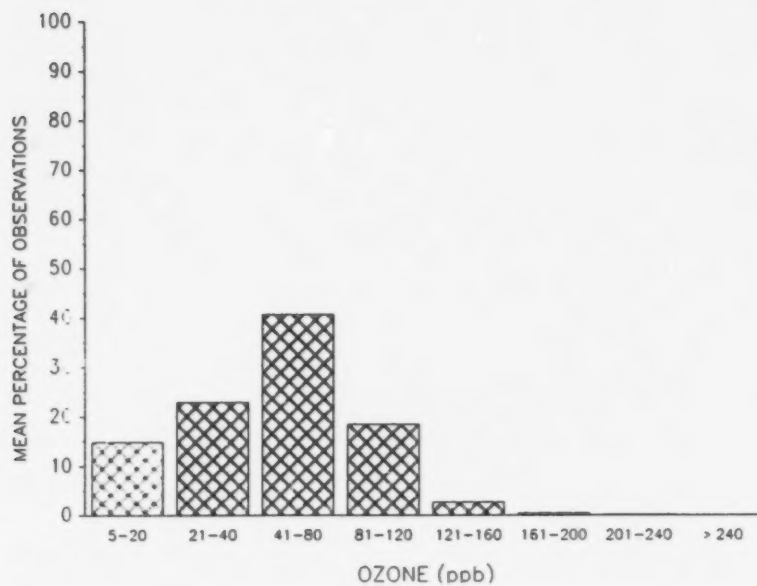


Figure 5.4. Histograms of observed and predicted daylight O₃ data for all stations in each of groups 1 through 6 for the period July 14–August 30, 1980.

SURFACE OZONE ANALYSIS GROUP TWO OBSERVED (DAYLIGHT HOURS)



SURFACE OZONE ANALYSIS GROUP TWO PREDICTED (DAYLIGHT HOURS)

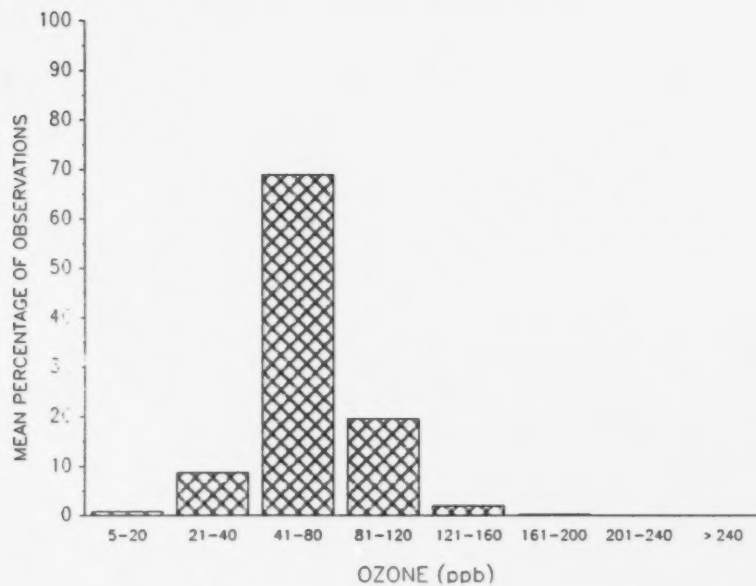
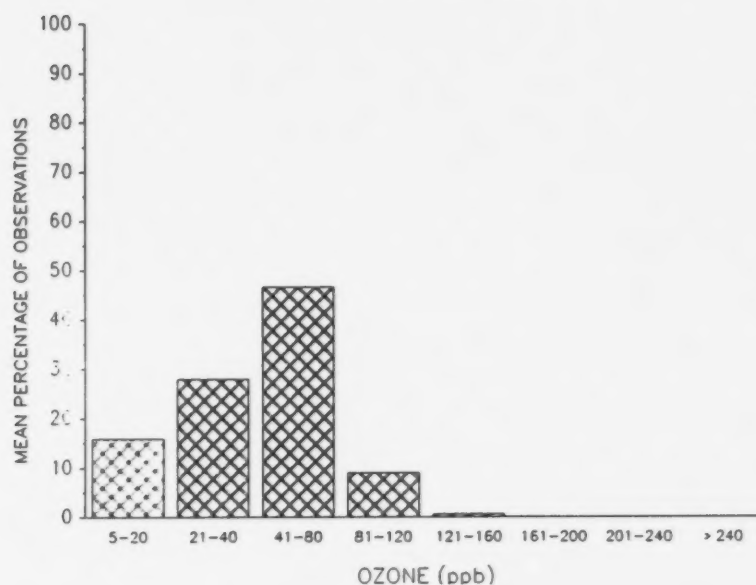


Figure 5.4. (continued)

SURFACE OZONE ANALYSIS

GROUP THREE OBSERVED (DAYLIGHT HOURS)



SURFACE OZONE ANALYSIS

GROUP THREE PREDICTED (DAYLIGHT HOURS)

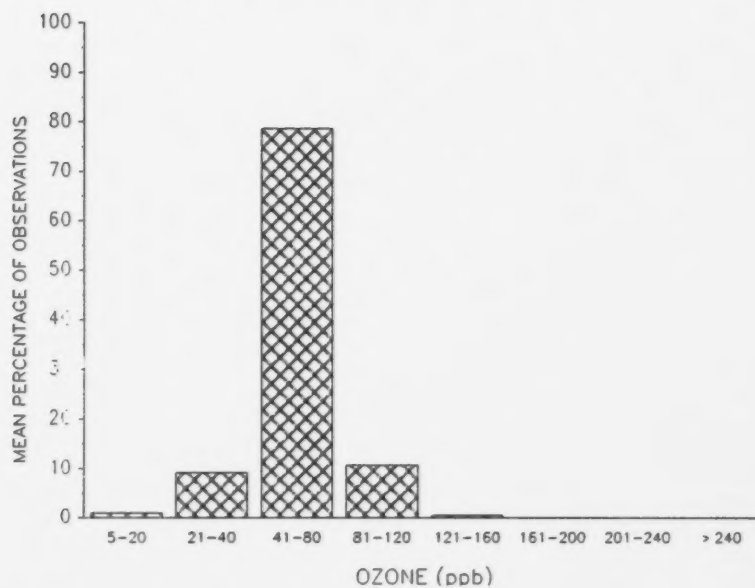
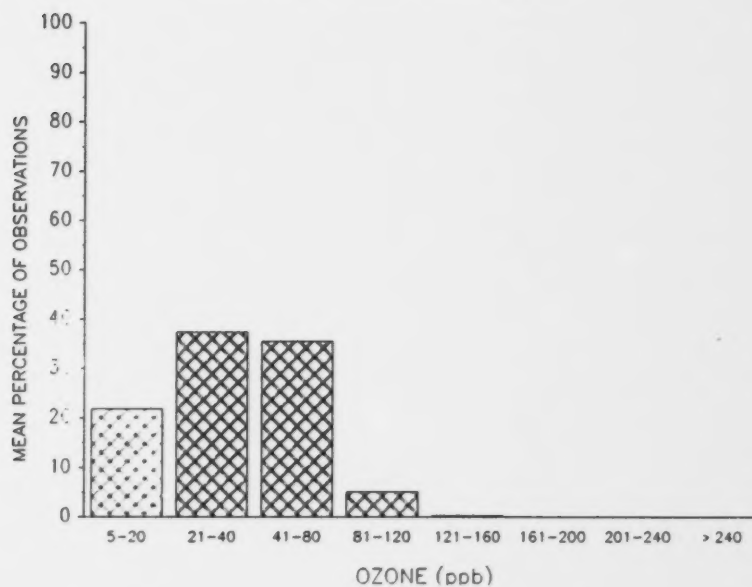


Figure 5.4. (continued)

SURFACE OZONE ANALYSIS

GROUP FOUR OBSERVED (DAYLIGHT HOURS)



SURFACE OZONE ANALYSIS

GROUP FOUR PREDICTED (DAYLIGHT HOURS)

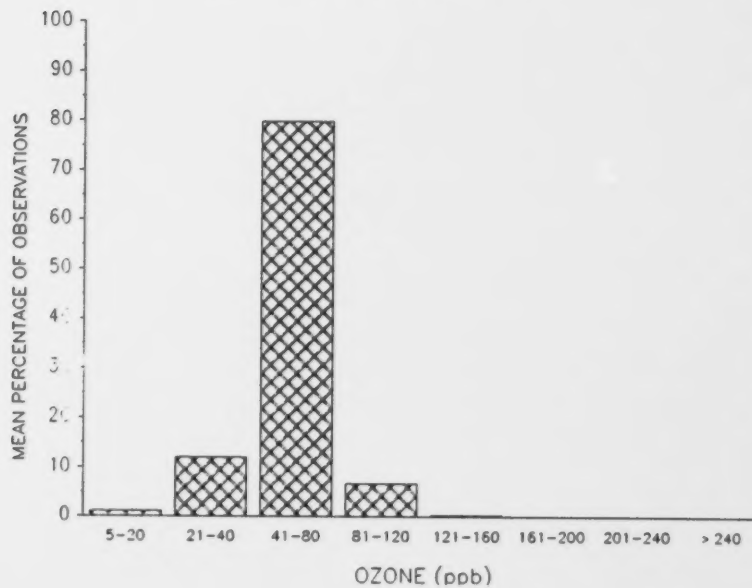
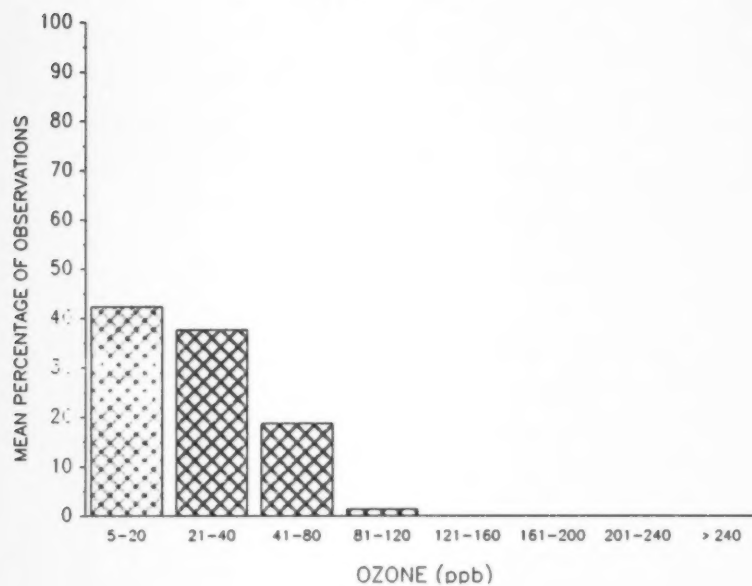


Figure 5.4. (continued)

SURFACE OZONE ANALYSIS GROUP FIVE OBSERVED (DAYLIGHT HOURS)



SURFACE OZONE ANALYSIS GROUP FIVE PREDICTED (DAYLIGHT HOURS)

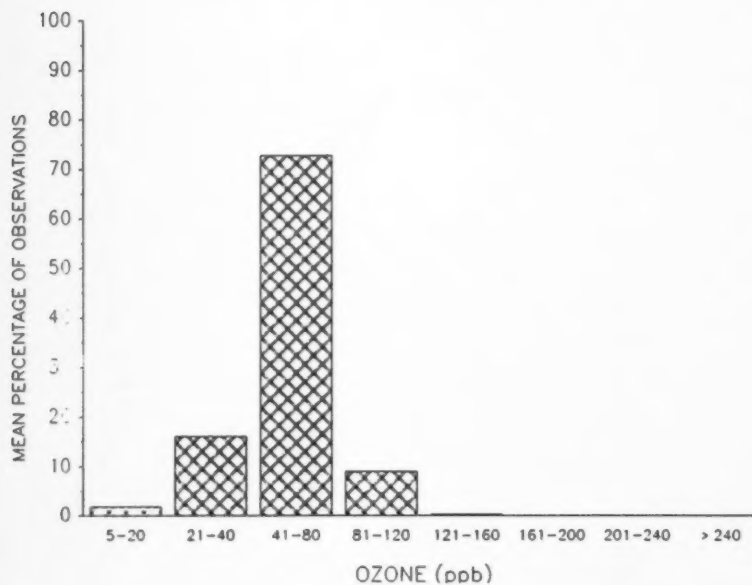
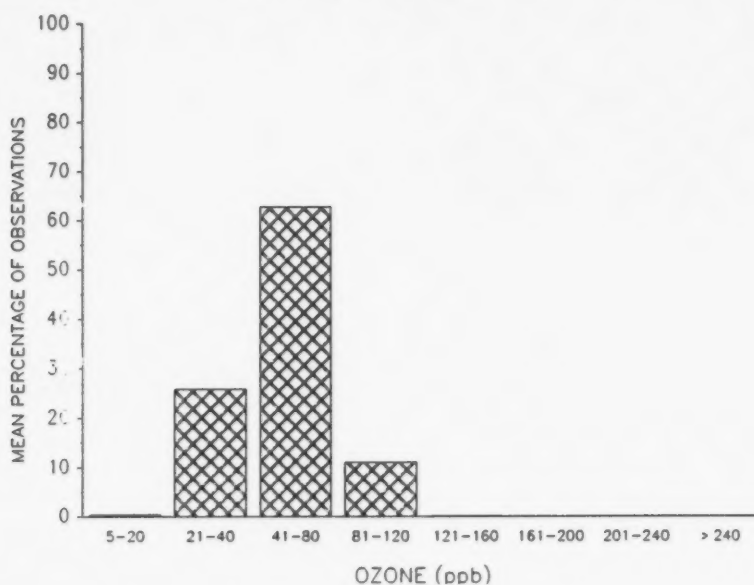


Figure 5.4. (continued)

SURFACE OZONE ANALYSIS

GROUP SIX OBSERVED (DAYLIGHT HOURS)



SURFACE OZONE ANALYSIS

GROUP SIX PREDICTED (DAYLIGHT HOURS)

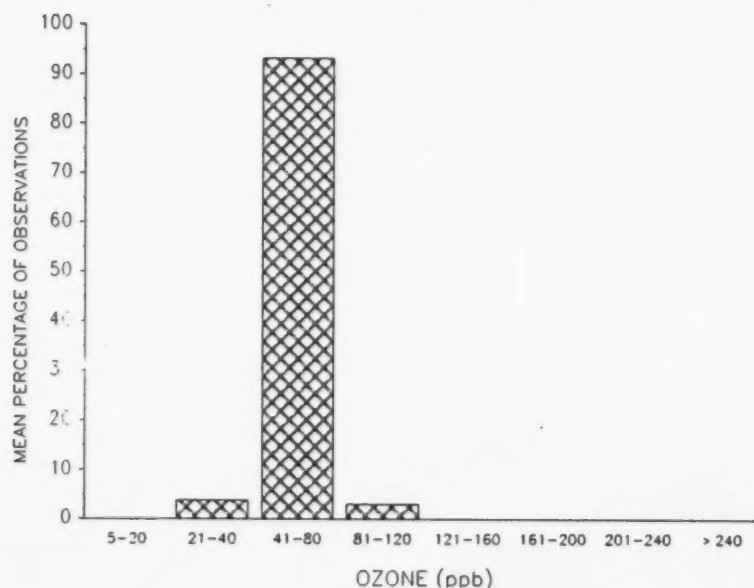


Figure 5.4. (continued)

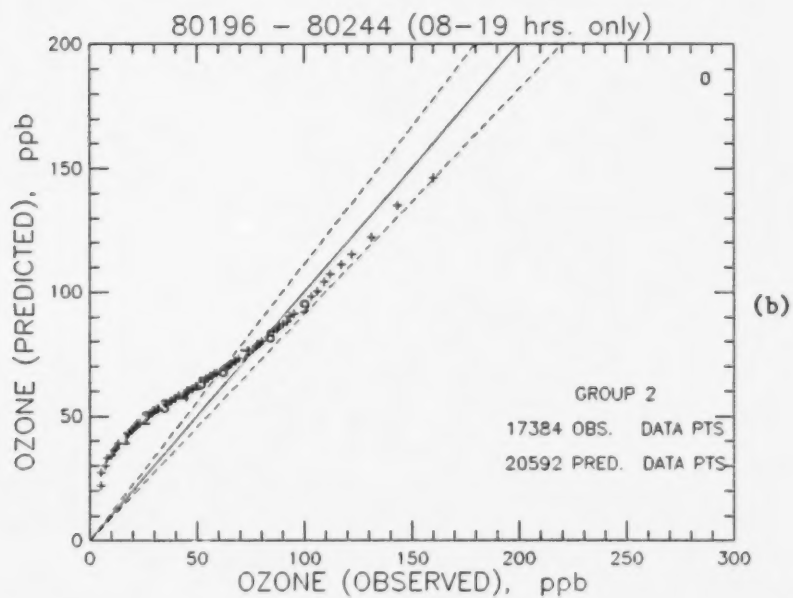
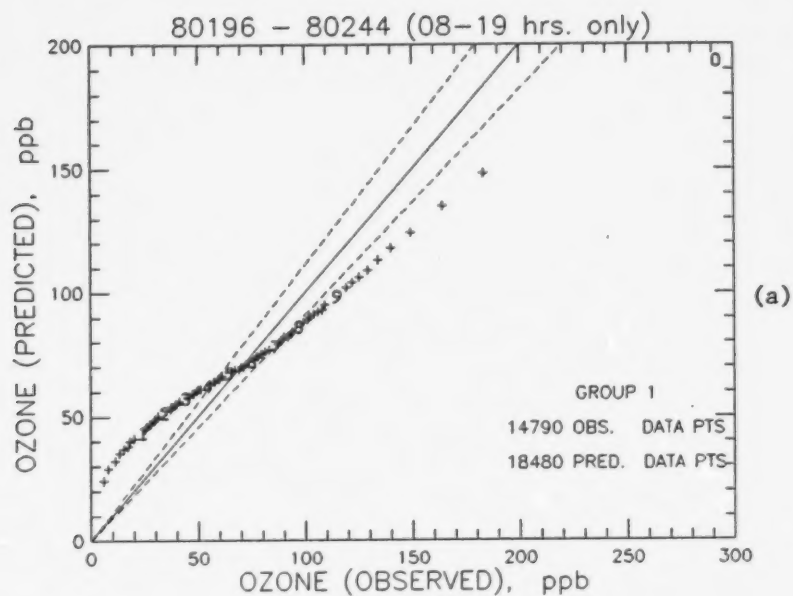


Figure 5.5. Cumulative frequency distributions of observed and predicted daytime hourly O_3 concentrations for groups 1-6 (a-f) over the period July 14-August 31, 1980. Each percentile level in the distribution is shown and every tenth level is indicated by an integer. The 99.5 percentile is also shown as the rightmost '+' in each figure.

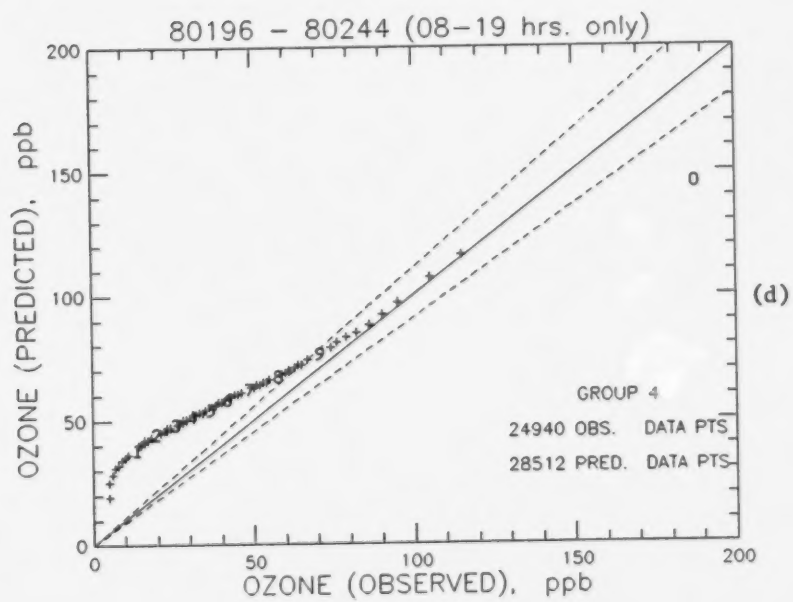
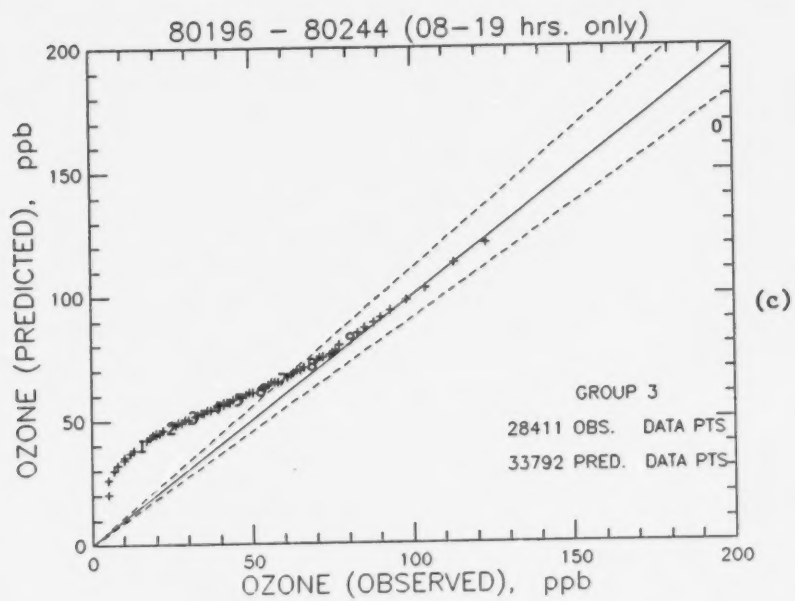


Figure 5.5. (continued)

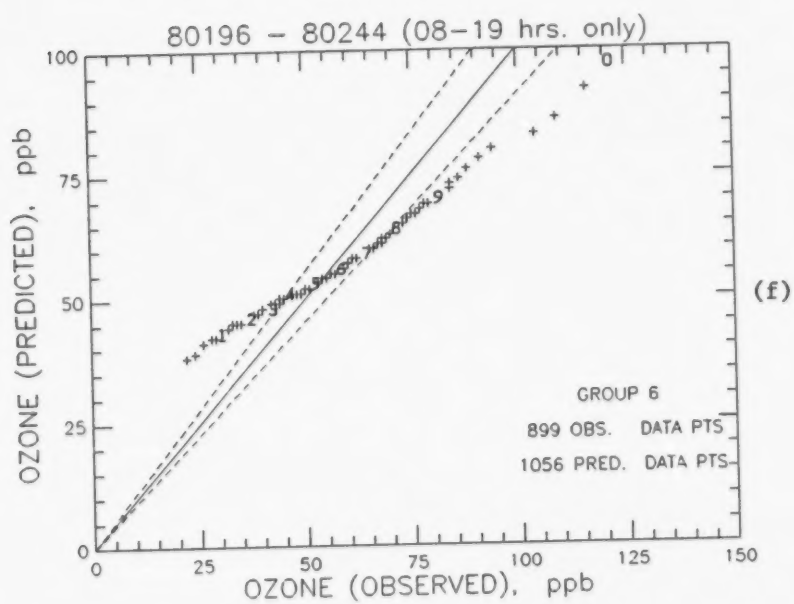
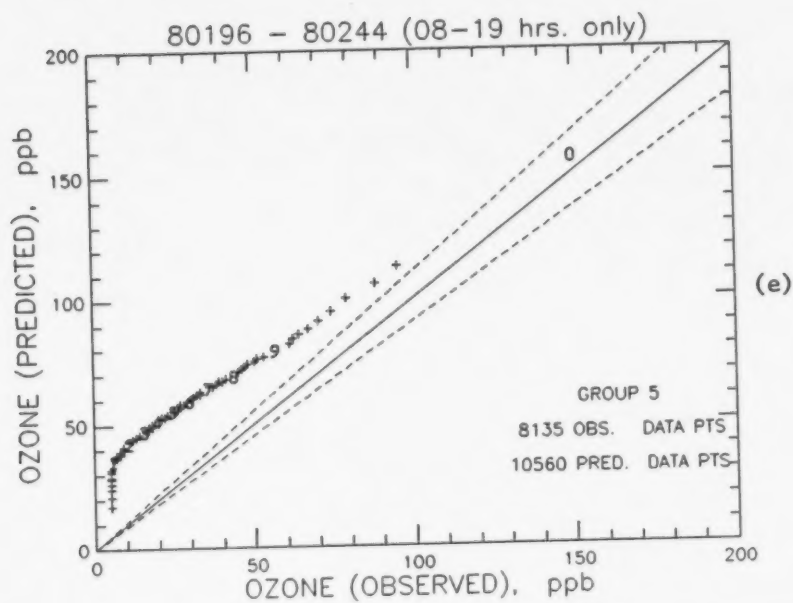
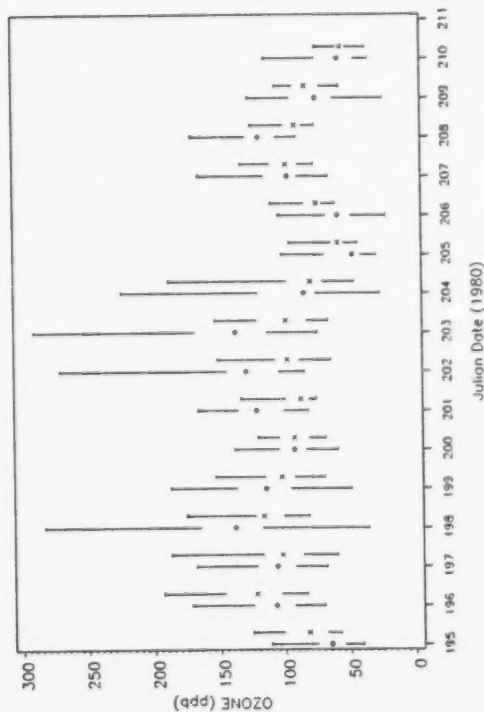
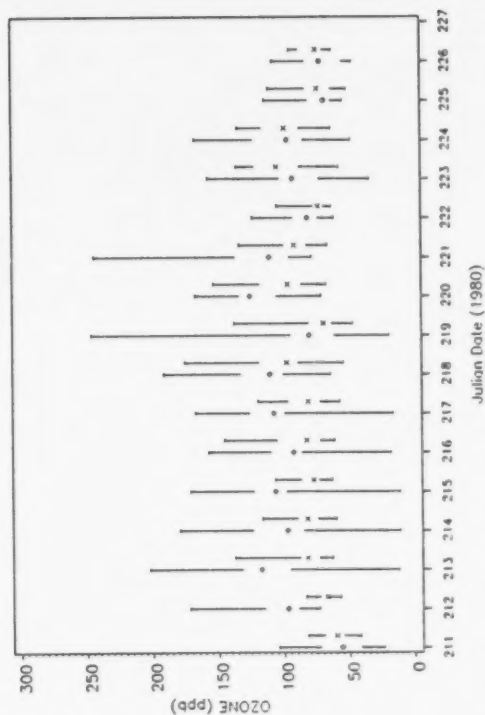


Figure 5.5. (continued)

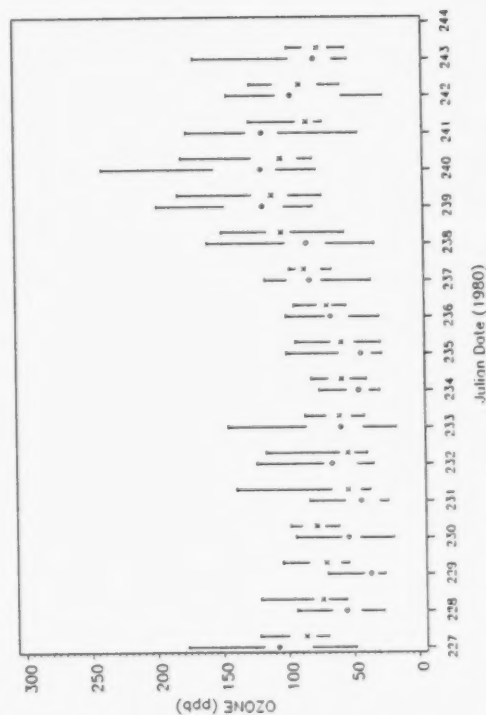
GROUP ONE (DAILY MAXIMUMS)
OBSERVED AND PREDICTED



GROUP ONE (DAILY MAXIMUMS)
OBSERVED AND PREDICTED



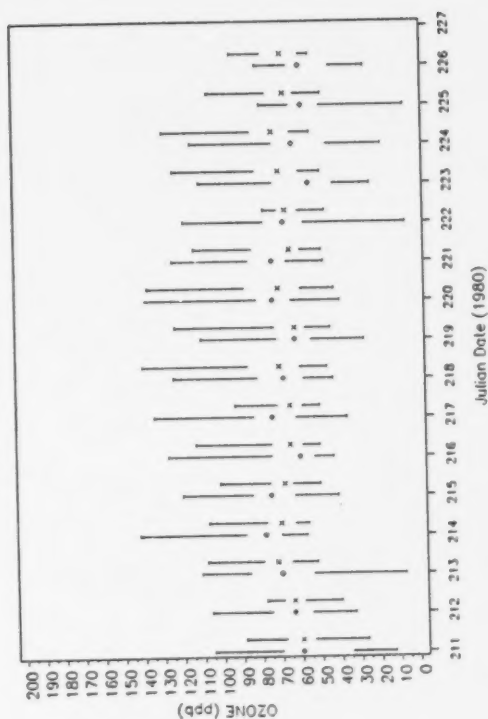
GROUP ONE (DAILY MAXIMUMS)
OBSERVED AND PREDICTED



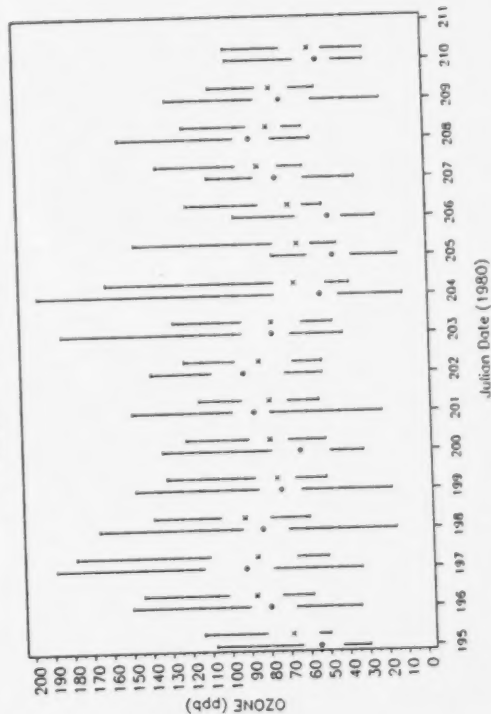
(a)

Figure 5.6. Time series of O_3 maxima, observed and predicted, for (a) group 1, (b) group 3, and (c) group 6. The median of the daily maximum value over all members of the group is shown (observed = diamonds, predicted = x's). The minimum, 25th, 75th, and maximum percentile points are also shown.

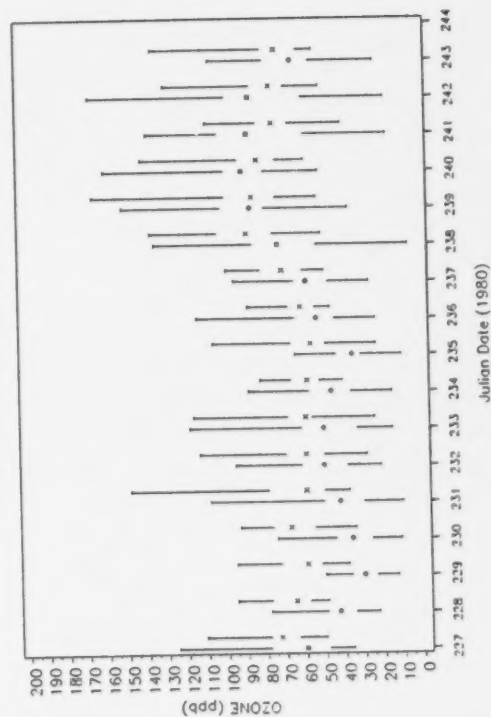
GROUP THREE (DAILY MAXIMUMS)
OBSERVED AND PREDICTED



GROUP THREE (DAILY MAXIMUMS)
OBSERVED AND PREDICTED

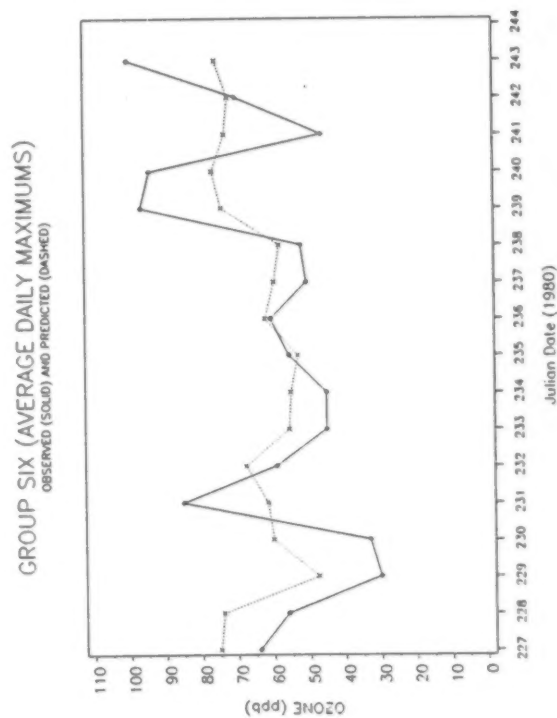
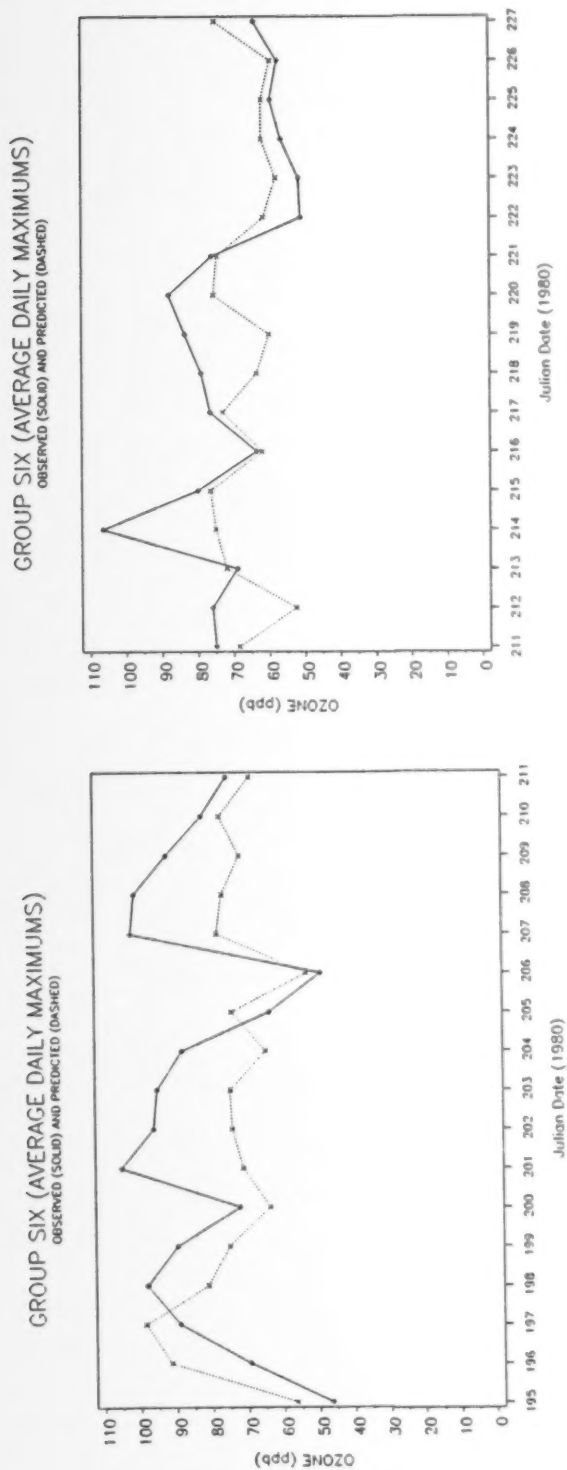


GROUP THREE (DAILY MAXIMUMS)
OBSERVED AND PREDICTED



(b)

Figure 5.6. (continued)



(c)

Figure 5.6. (continued)

MAXIMUM HOURLY OZONE CONCENTRATION
DAILY MEDIAN PLUS/MINUS 95% C.I.
OBSERVED (o) AND PREDICTED (x)

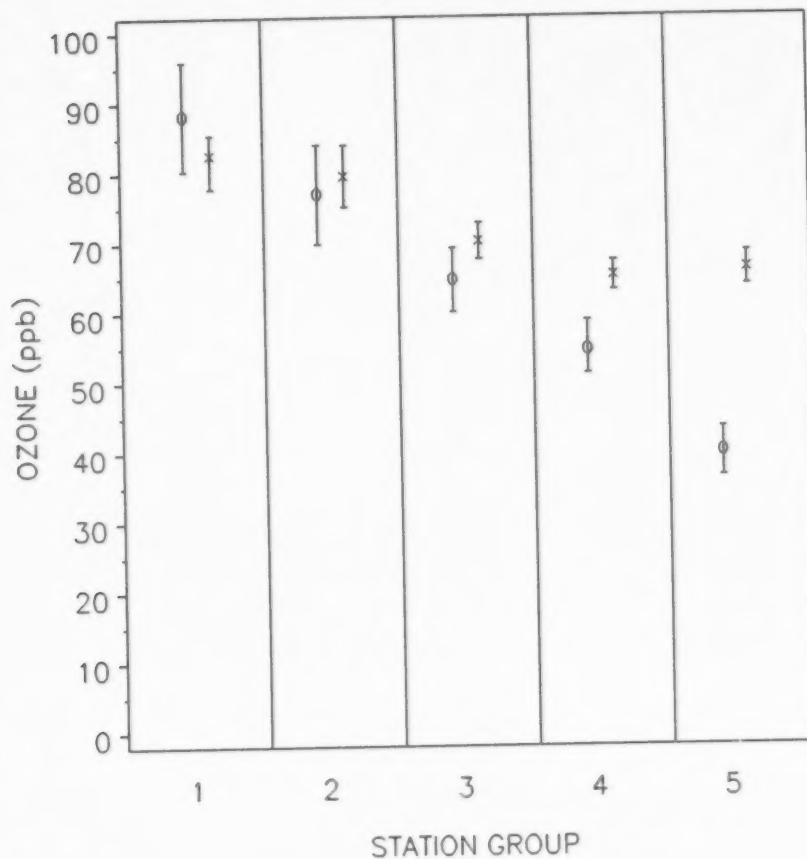
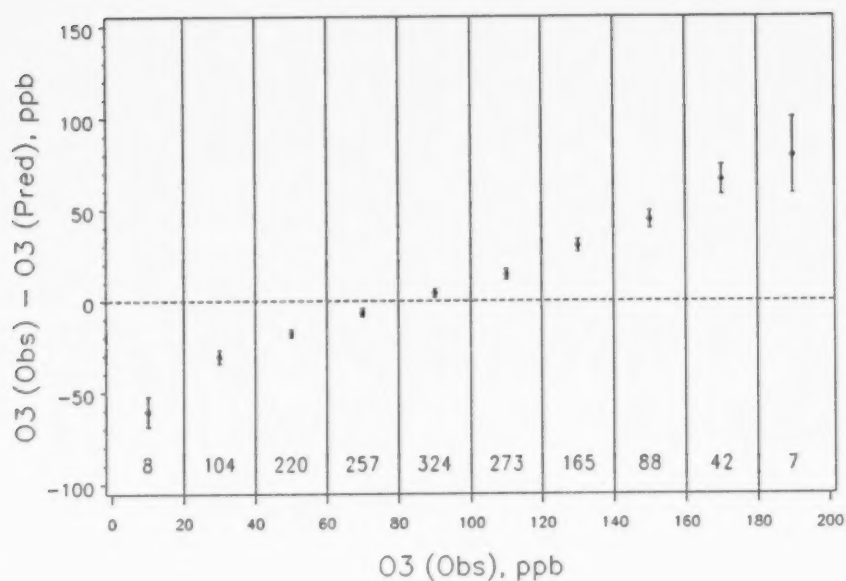


Figure 5.7. Average and 95% confidence limits of median of O_3 maxima for groups 1-5 over the period July 14-August 31, 1980. Observed values are indicated by o's and predicted values by x's.

BIAS VS. OBSERVED CONCENTRATION – GROUP 1
MAXIMUM DAILY OZONE



BIAS VS. OBSERVED CONCENTRATION – GROUP 2
MAXIMUM DAILY OZONE

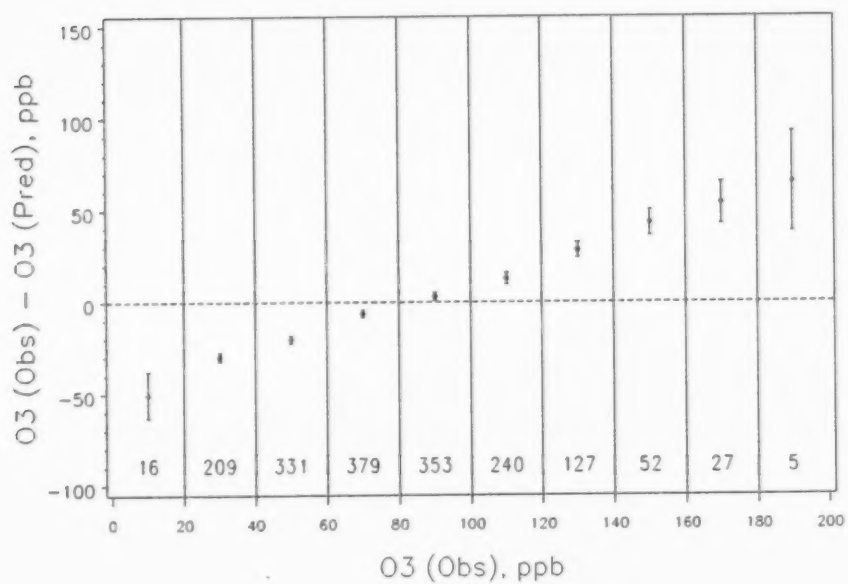
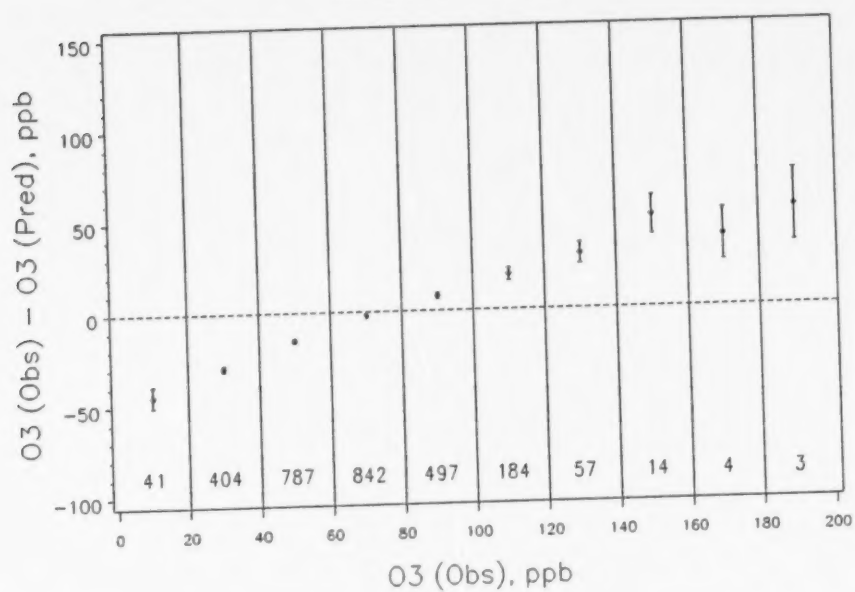


Figure 5.8. Bias vs. observed concentration for maximum daily O_3 over the simulation period July 14–August 31, 1980 for groups 1 through 6. The 95% confidence interval is shown about the mean value for each concentration interval.

BIAS VS. OBSERVED CONCENTRATION - GROUP3
MAXIMUM DAILY OZONE



BIAS VS. OBSERVED CONCENTRATION - GROUP4
MAXIMUM DAILY OZONE

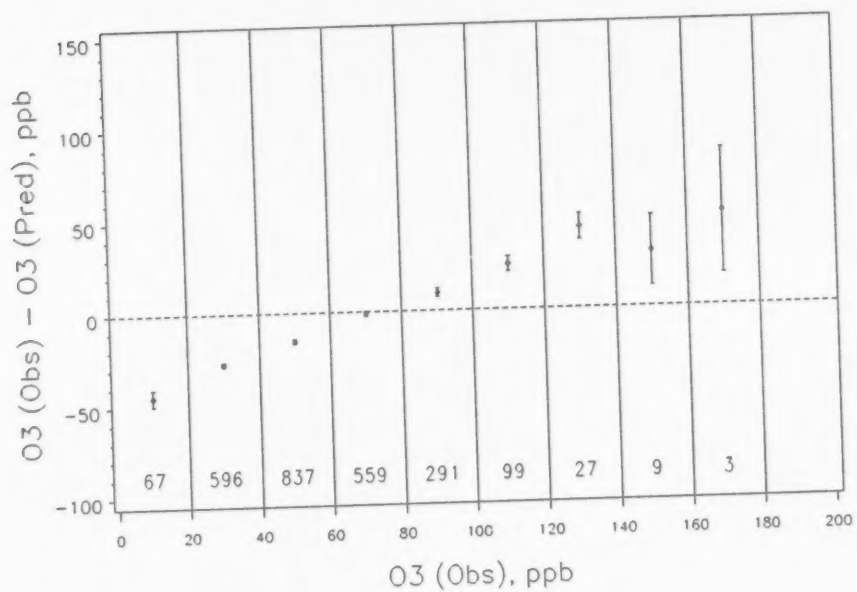
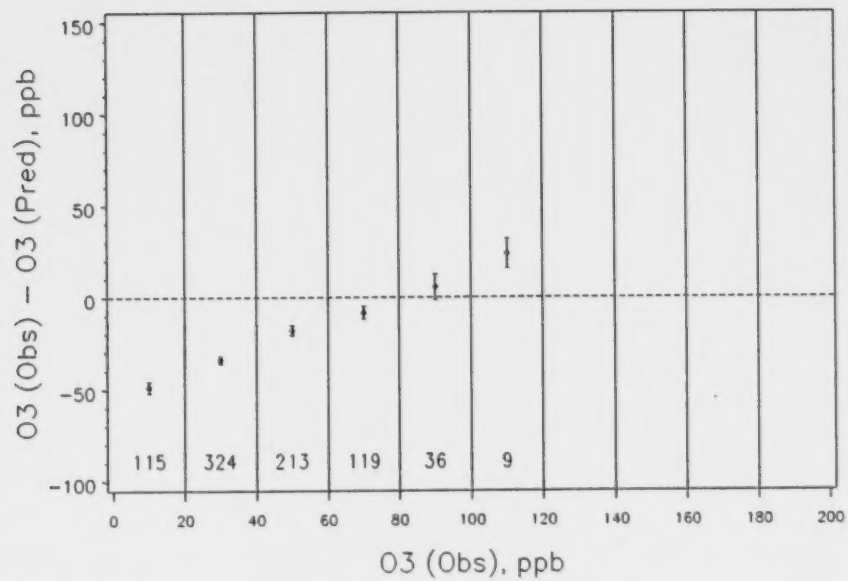


Figure 5.8. (continued)

BIAS VS. OBSERVED CONCENTRATION – GROUP5
MAXIMUM DAILY OZONE



BIAS VS. OBSERVED CONCENTRATION – GROUP6
MAXIMUM DAILY OZONE

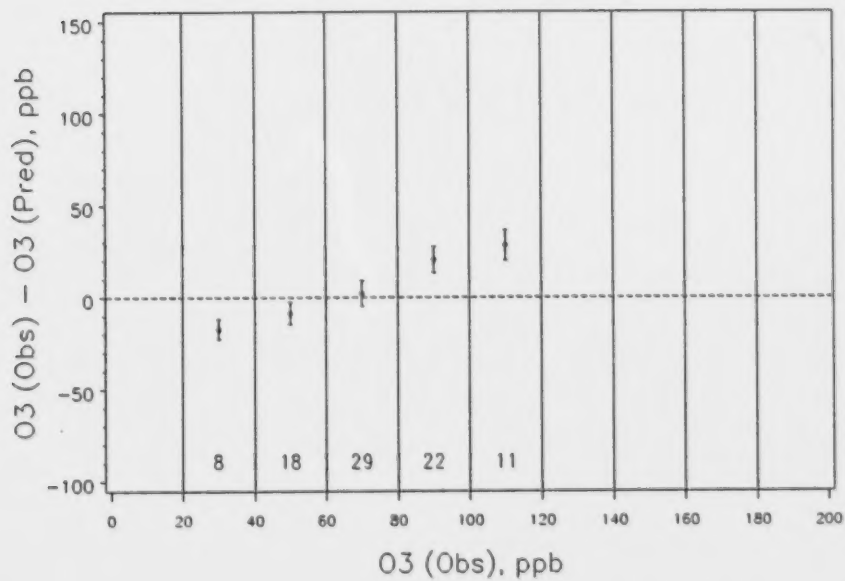
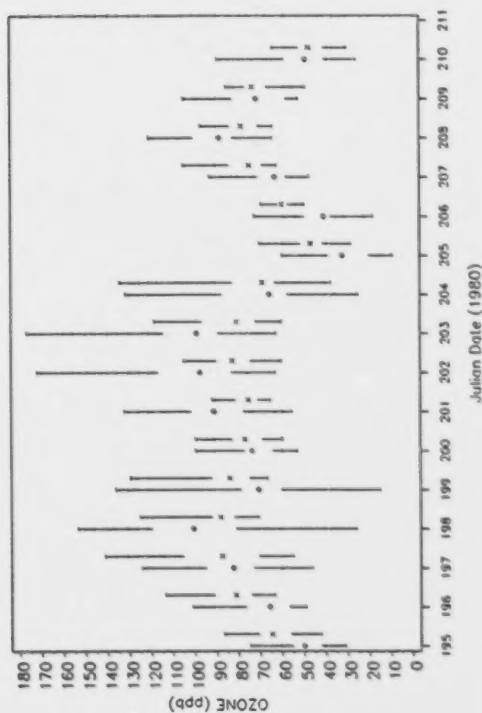
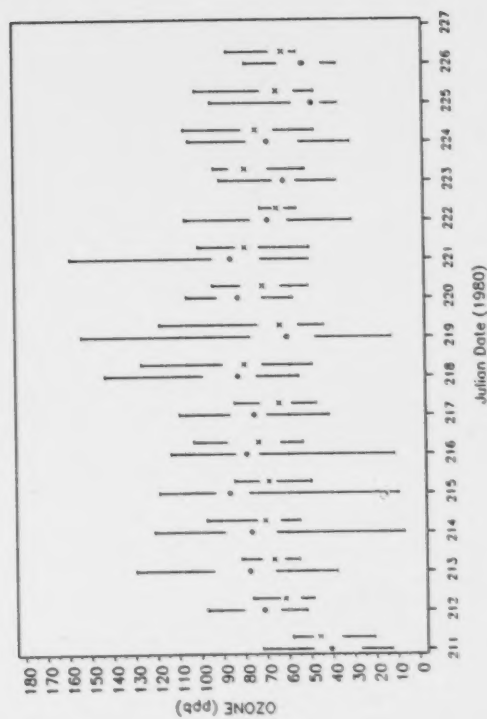


Figure 5.8. (continued)

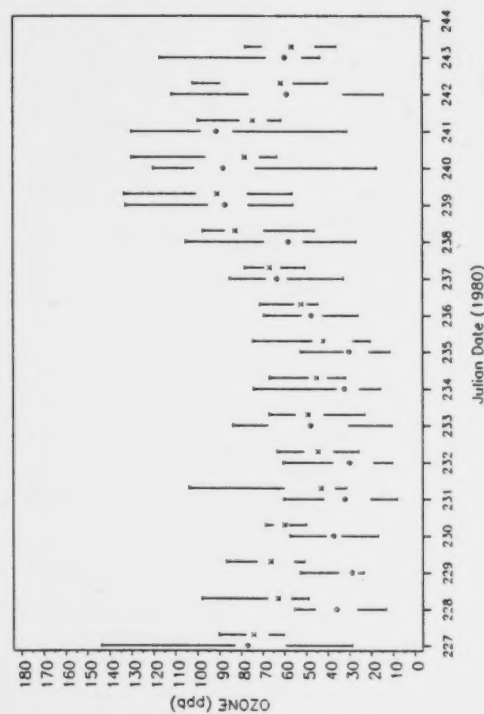
GROUP ONE (SEVEN HOUR AVERAGES)
OBSERVED AND PREDICTED



GROUP ONE (SEVEN HOUR AVERAGES)
OBSERVED AND PREDICTED



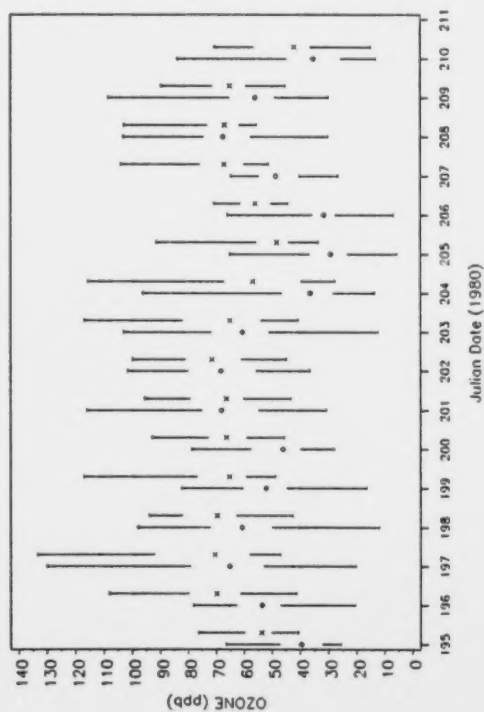
GROUP ONE (SEVEN HOUR AVERAGES)
OBSERVED AND PREDICTED



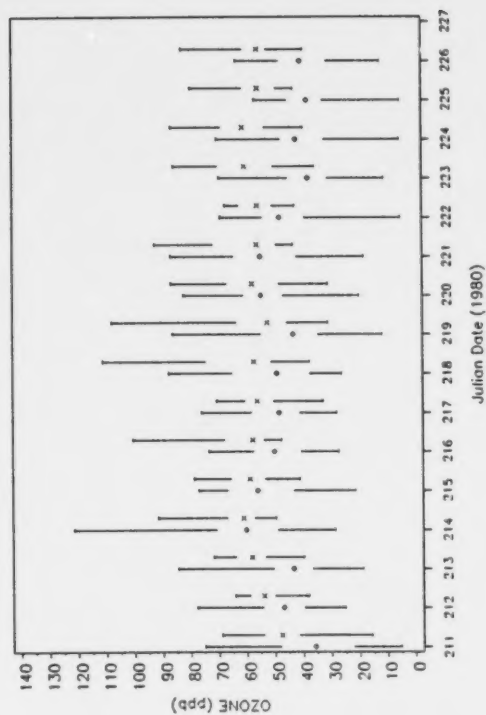
(a)

Figure 5.9. Time series of 7-hr (09-16 h, LST) average O_3 , observed and predicted, for (a) group 1, (b) group 3, and (c) group 6. The median of the daily 7-hr average value over all members of the group is shown (observed = diamonds, predicted = x's). The minimum, 25th, 75th, and maximum percentile points are also shown.

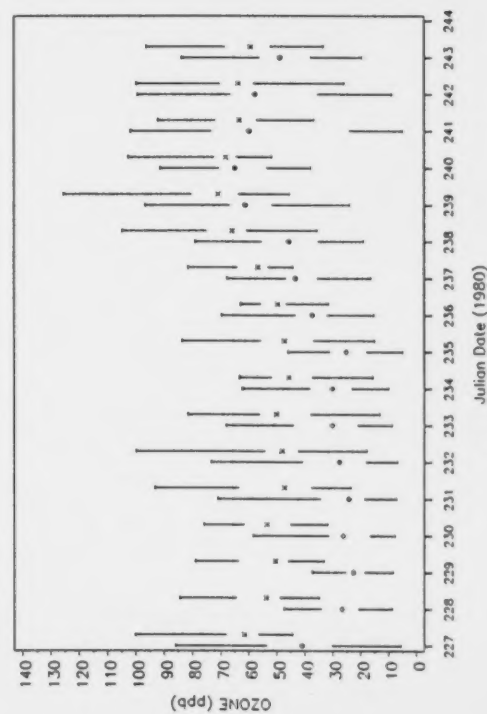
GROUP THREE (SEVEN HOUR AVERAGES)
OBSERVED AND PREDICTED



GROUP THREE (SEVEN HOUR AVERAGES)
OBSERVED AND PREDICTED



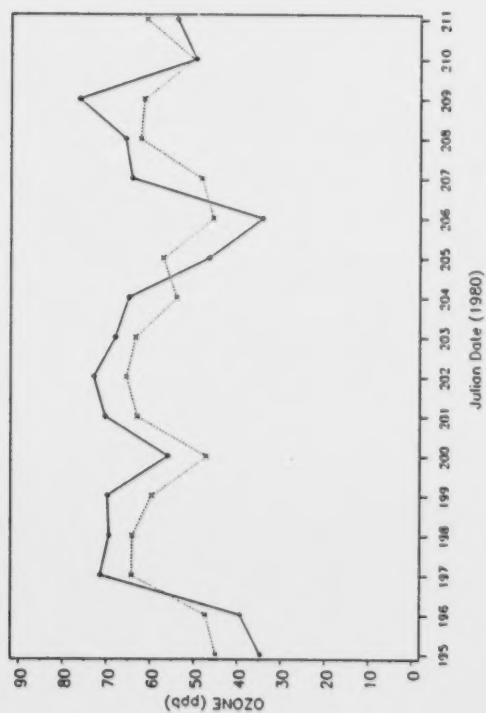
GROUP THREE (SEVEN HOUR AVERAGES)
OBSERVED AND PREDICTED



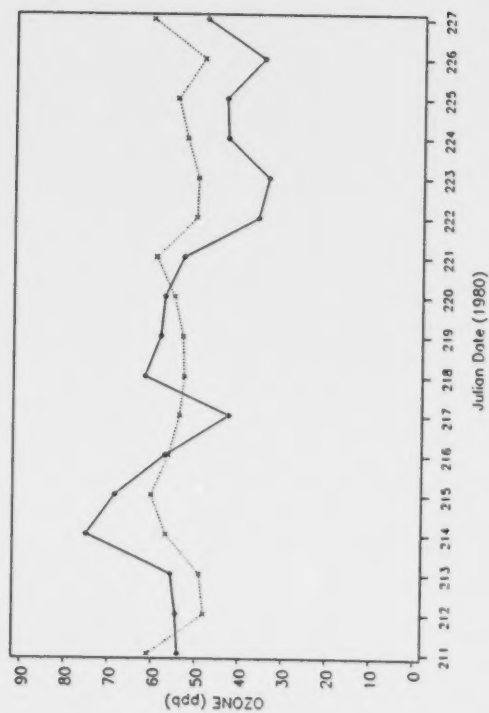
(b)

Figure 5.9. (continued)

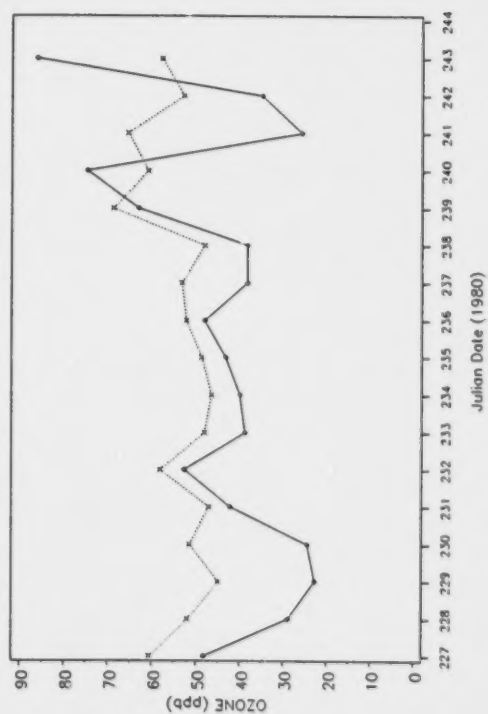
GROUP SIX (SEVEN HOUR AVERAGES)
OBSERVED (SOLID) AND PREDICTED (DASHED)



GROUP SIX (SEVEN HOUR AVERAGES)
OBSERVED (SOLID) AND PREDICTED (DASHED)



GROUP SIX (SEVEN HOUR AVERAGES)
OBSERVED (SOLID) AND PREDICTED (DASHED)



(c)

Figure 5.9. (continued)

7-HOUR AVERAGE OZONE CONCENTRATION
DAILY MEDIAN PLUS/MINUS 95% C.I.
OBSERVED (o) AND PREDICTED (x)

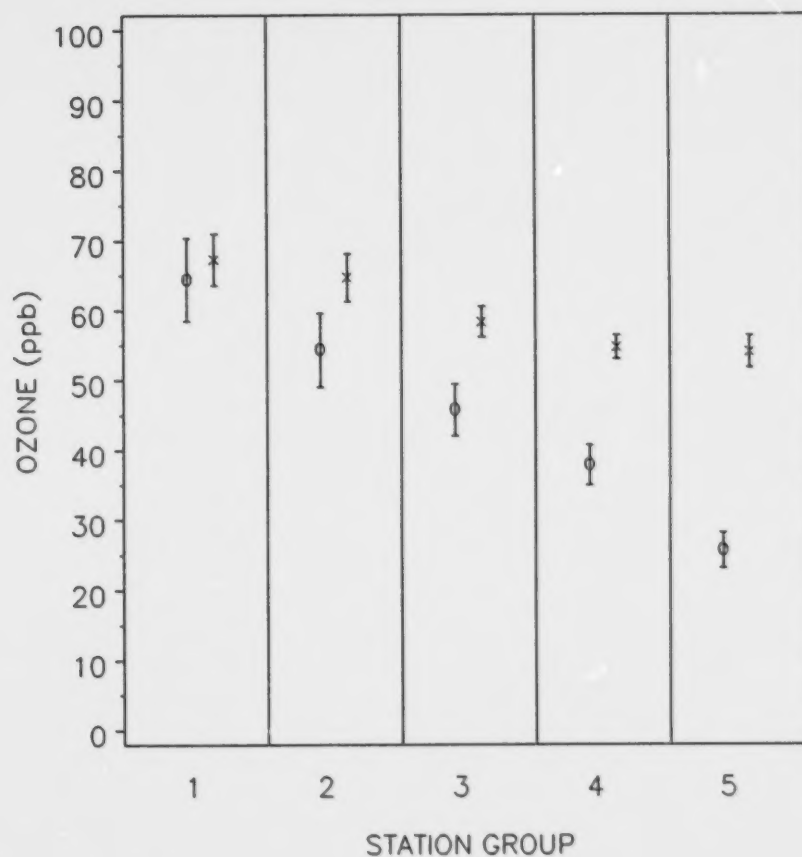
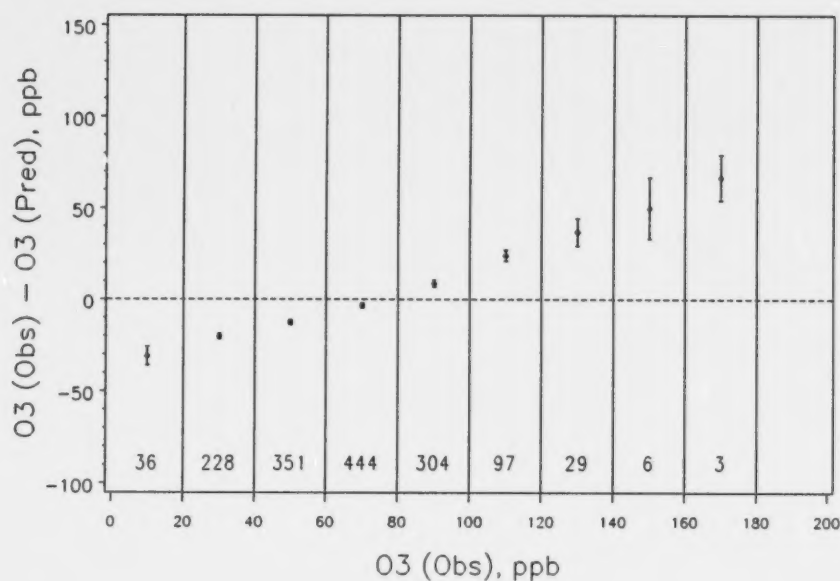


Figure 5.10. Average and 95% confidence limits of median of 7-hr (09-16 h, LST) average O_3 for groups 1-5 over the period July 14-August 31, 1980. Observed values are indicated by o's and predicted values by x's.

BIAS VS. OBSERVED CONCENTRATION - GROUP 1
7-HOUR (0900-1500) AVERAGE OZONE



BIAS VS. OBSERVED CONCENTRATION - GROUP 2
7-HOUR (0900-1500) AVERAGE OZONE

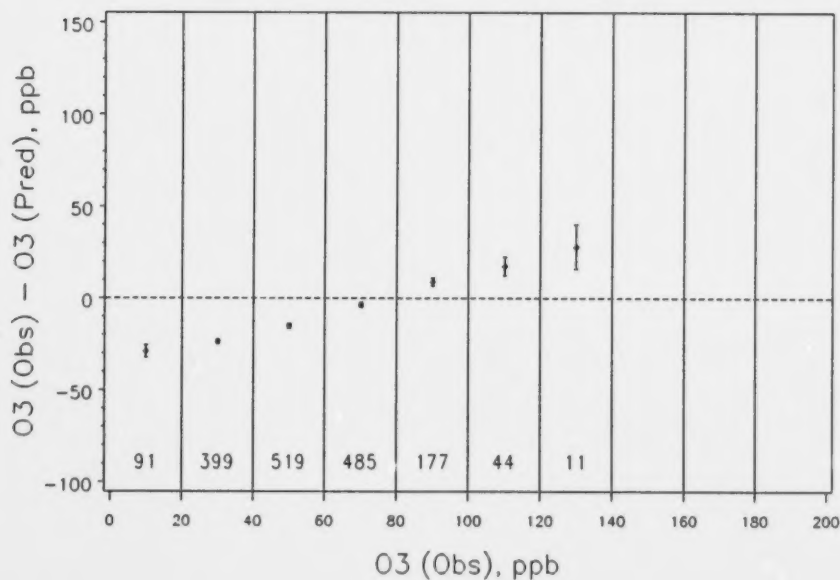
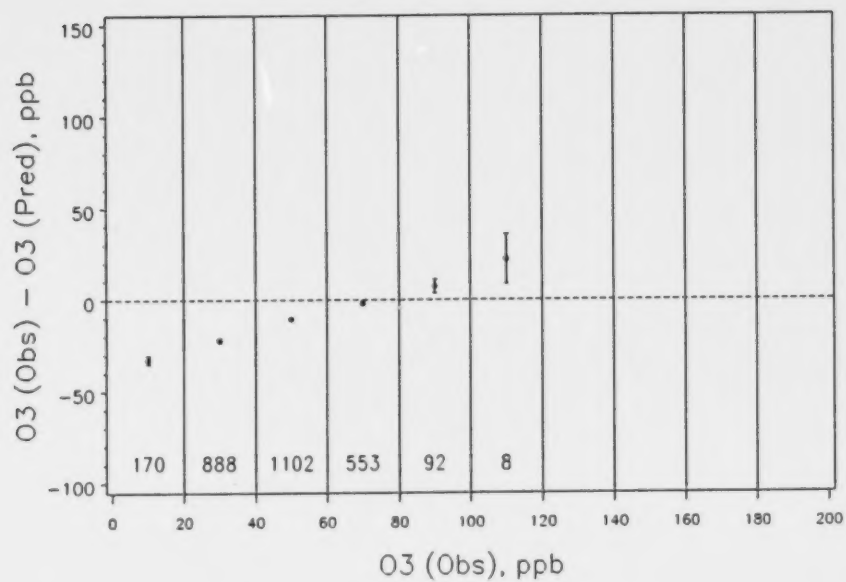


Figure 5.11. Bias vs. observed concentration for 7-hr average (09-16 h, LST) daily O_3 over the simulation period July 14-August 31, 1980 for groups 1 through 6. The 95% confidence interval is shown about the mean value for each concentration interval.

BIAS VS. OBSERVED CONCENTRATION - GROUP3
7-HOUR (0900-1500) AVERAGE OZONE



BIAS VS. OBSERVED CONCENTRATION - GROUP4
7-HOUR (0900-1500) AVERAGE OZONE

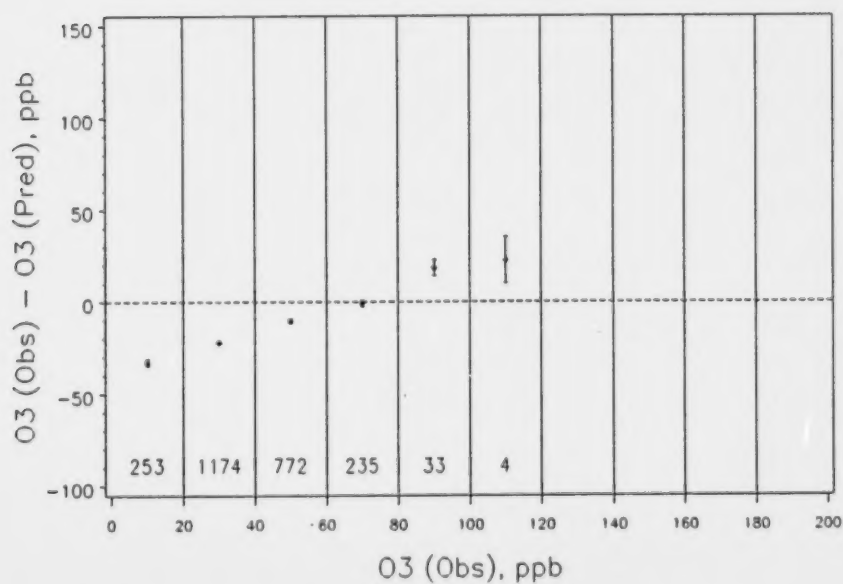
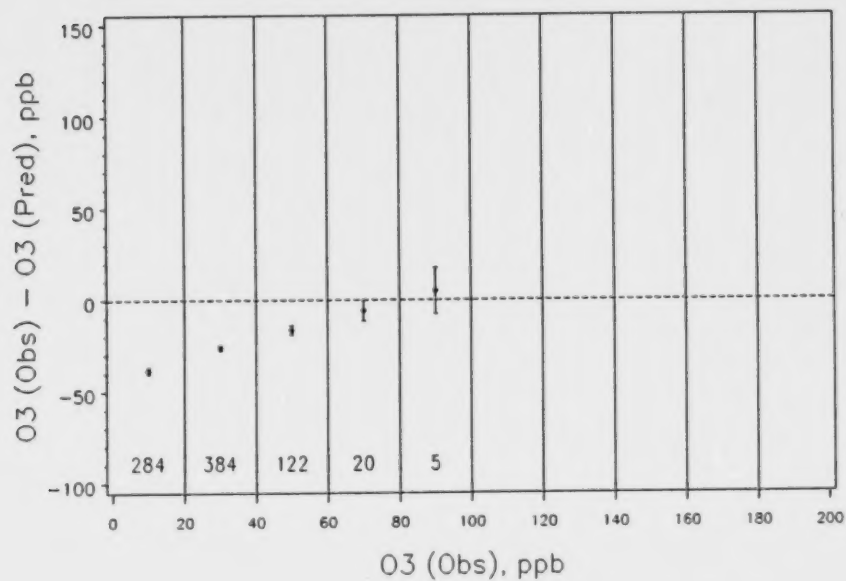


Figure 5.11. (continued)

BIAS VS. OBSERVED CONCENTRATION - GROUP5
7-HOUR (0900-1500) AVERAGE OZONE



BIAS VS. OBSERVED CONCENTRATION - GROUP6
7-HOUR (0900-1500) AVERAGE OZONE

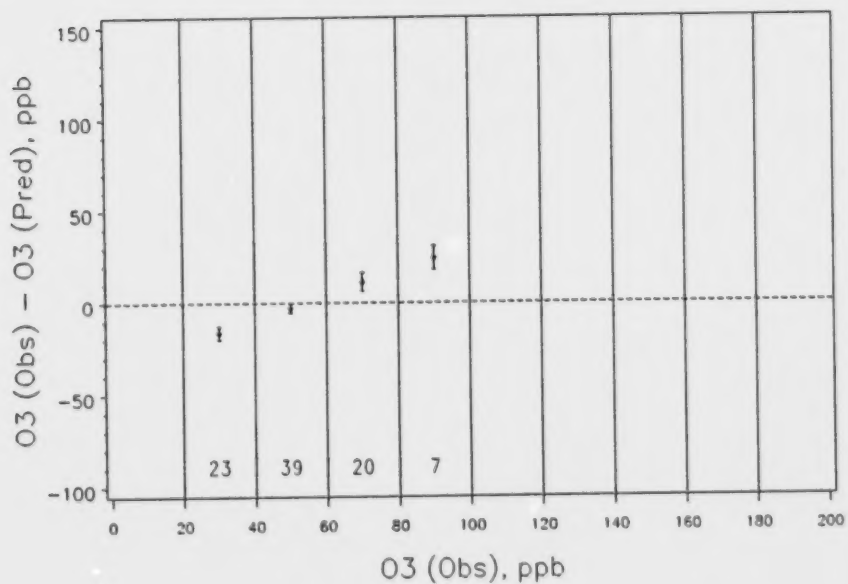


Figure 5.11. (continued)

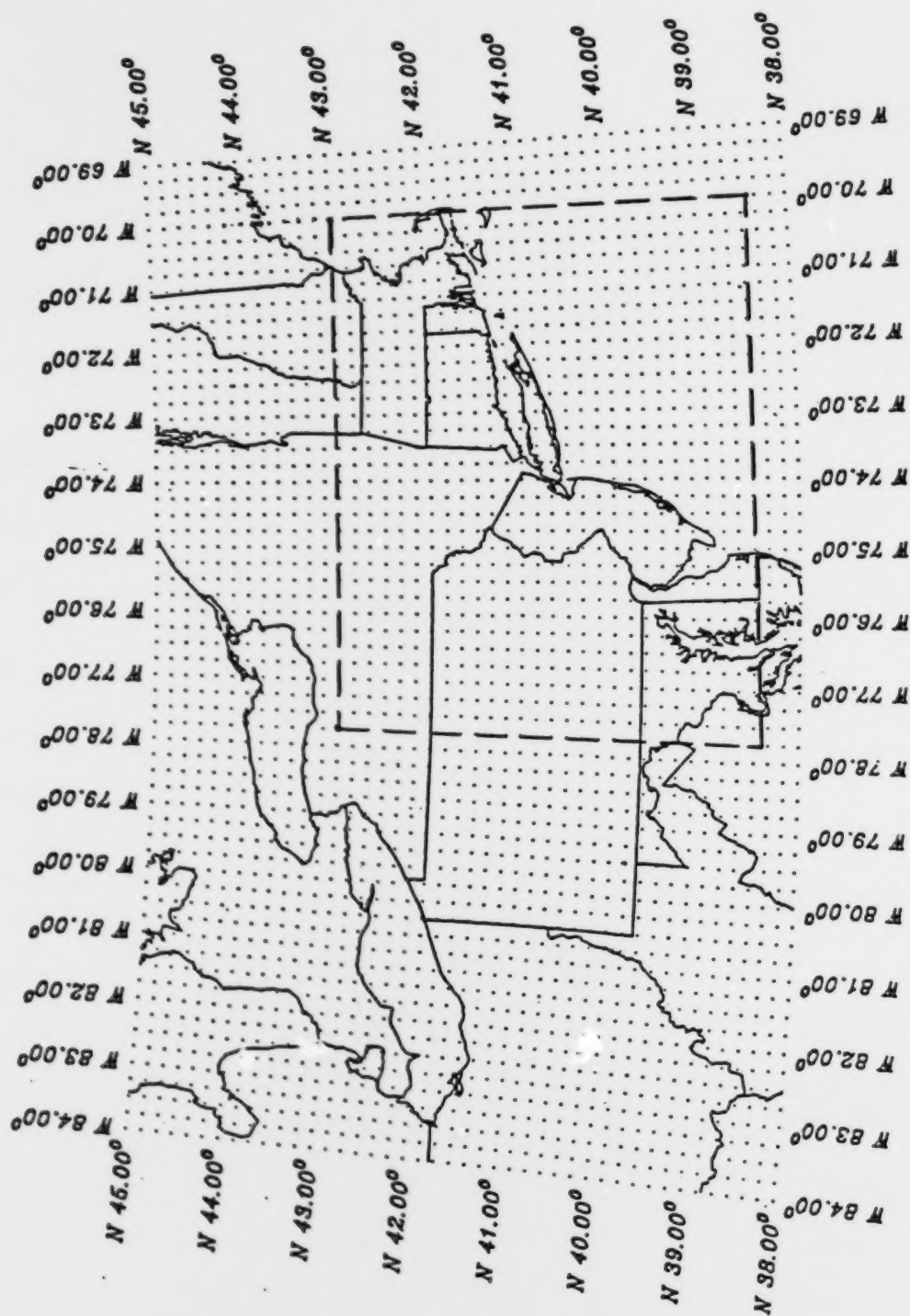


Figure 5.12. Relationship of subregion to full ROM domain.

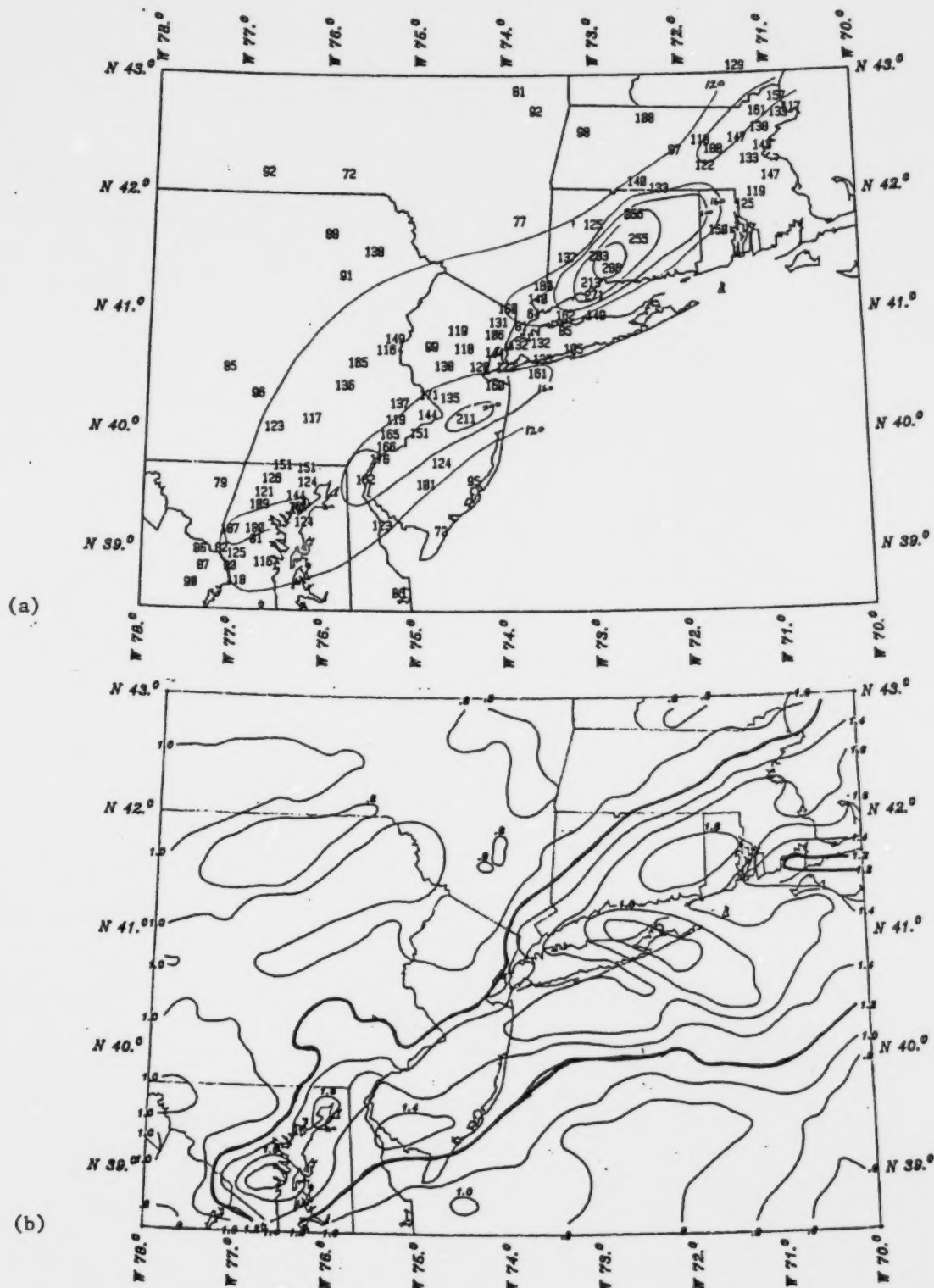


Figure 5.13. Contours of maximum hourly O_3 concentrations over the period July 14-17, 1980 for (a) observed and (b) predicted data sets. Contours of observed data are in concentration units of ppb and contours of predicted data are in units of ppb/100.

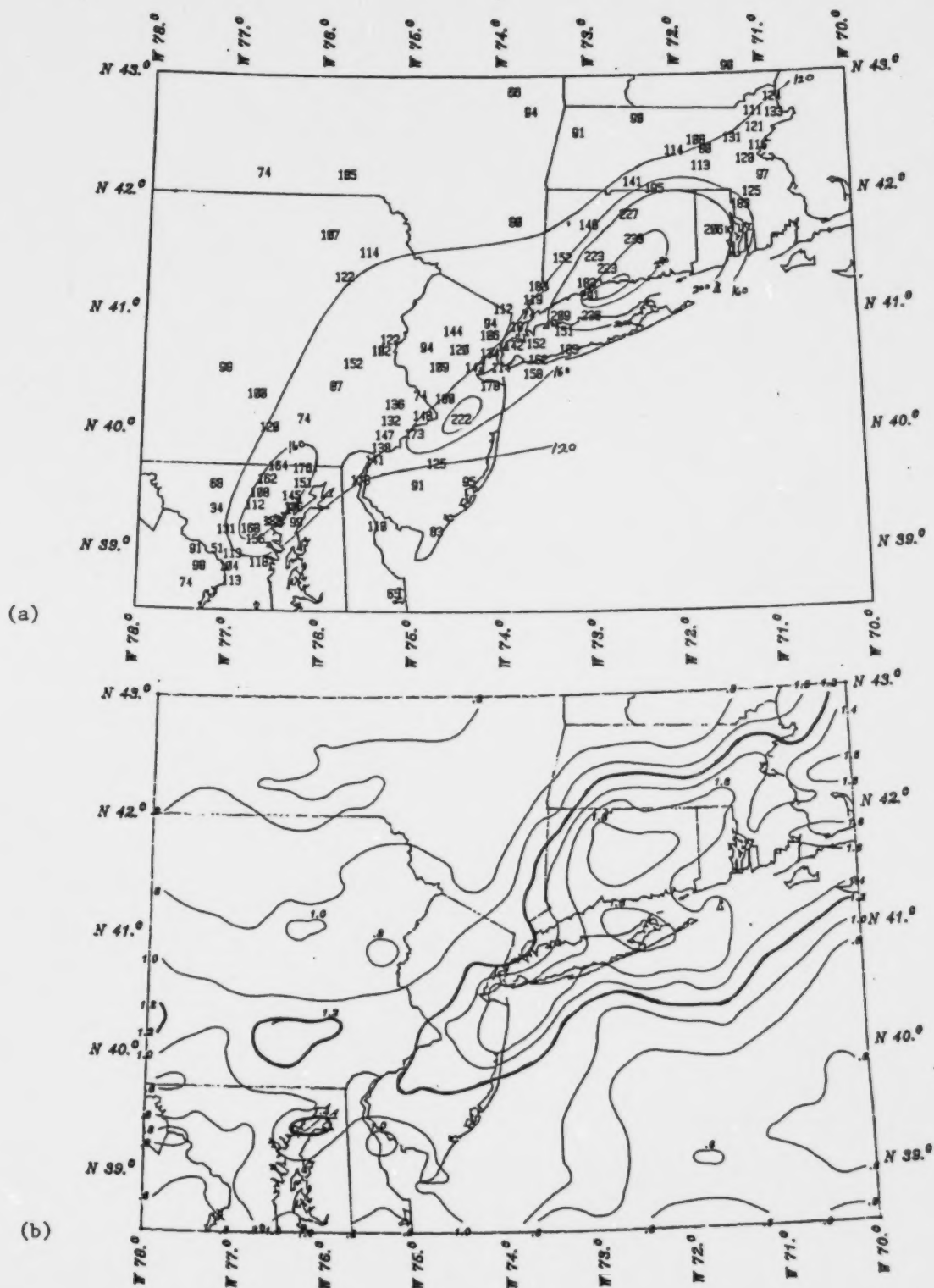


Figure 5.14. Contours of maximum hourly O_3 concentrations over the period July 20-22, 1980 for (a) observed and (b) predicted data sets. Contours of observed data are in concentration units of ppb and contours of predicted data are in units of ppb/100.

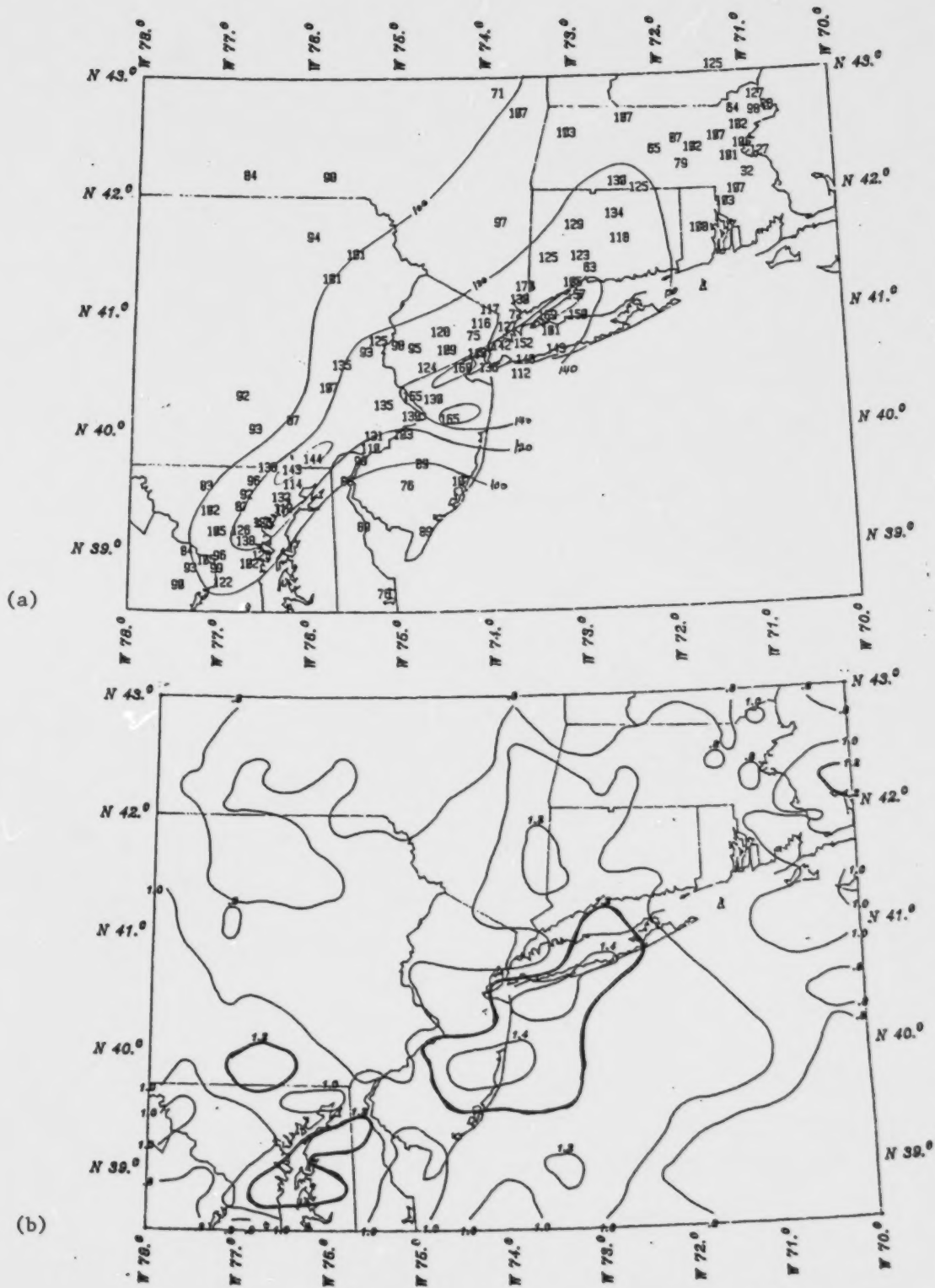


Figure 5.15. Contours of maximum hourly O_3 concentrations over the period July 25-27, 1980 for (a) observed and (b) predicted data sets. Contours of observed data are in concentration units of ppb and contours of predicted data are in units of ppb/100.

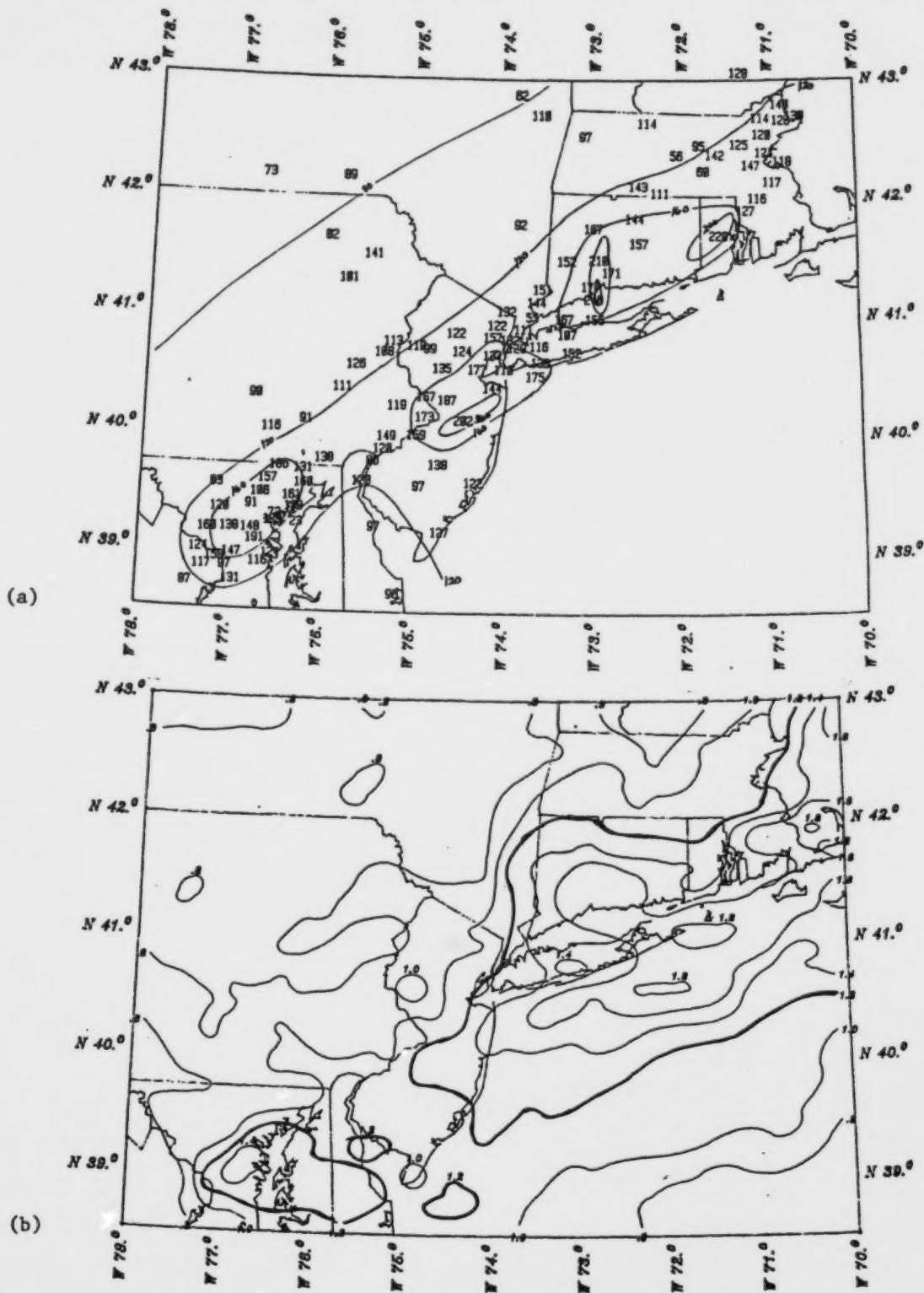


Figure 5.16. Contours of maximum hourly O_3 concentrations over the period July 30–August 8, 1980 for (a) observed and (b) predicted data sets. Contours of observed data are in concentration units of ppb and contours of predicted data are in units of ppb/100.

6 EVALUATION OF SURFACE NO_x AND NO_2

6.1 DATA PREPARATION

6.1.1 Surface Monitoring Network

Air quality monitoring for NO_x and NO_2 is generally not as extensive as that for O_3 in the U.S. During the 1980 simulation period discussed here there were 65 active monitoring sites for NO_x and 107 for NO_2 in the portions of the SAROAD and Canadian networks contained in the ROM domain. As with O_3 , nearly all of the sites were located within urban areas. Figures 6.1 and 6.2 show the grid cells within the ROM domain where the NO_x and NO_2 monitoring sites were located and Tables 6.1 and 6.2 list each of the stations and their locations.

Using this network to verify the performance of the ROM for predicting NO_x and NO_2 concentrations poses several problems. The greatest problem is that the nature of these chemical species in the atmosphere is largely *primary*, that is, the flux of emissions of the species is generally the largest contributor to the ambient concentrations. This being the case, the large spatial variations in emissions patterns are expected to produce large spatial variations in ambient concentrations, especially on the urban scale where the emissions heterogeneity is greatest. Urban-oriented monitors, such as those available here for NO_x and NO_2 , will capture concentration patterns characteristic of the local area only. Monitors located in rural areas, or areas that might be more regionally representative, were generally not available in 1980.

Comparison of ROM predictions of NO_x and NO_2 resolved to the 18.5 km grid resolution can not be compared very well with measurements from one or two monitoring sites within an urban area because of this scale problem and the primary nature of the species. Similar scale problems exist for O_3 , as discussed in the previous section, but are mitigated somewhat by the *secondary* nature of the pollutant and its smaller spatial concentration gradients. The discussion that

TABLE 6.1. NOx MONITORING STATIONS - NEROS REGION - 1980

I.D.	Location	State	Lat. (deg.,N)	Lon. (deg.,W)	ROM Grid x	Cell y
GRV	GREENWICH	CT	41.0794	73.7053	42	19
HF2	HARTFORD	CT	41.7608	72.6789	46	23
DC1	WASHINGTON	DC	38.9036	77.0517	28	6
BS3	BOSTON	MA	42.3781	71.0283	52	27
DVR	DANVERS	MA	42.5919	70.9769	53	28
EST	EASTON	MA	42.0672	71.0906	52	25
MED	MEDFIELD	MA	42.2122	71.3356	51	26
SOM	SOMERVILLE	MA	42.4036	71.1083	52	27
TEW	TEWKSBURY	MA	42.6081	71.2206	52	28
BL1	BALTIMORE	MD	39.2997	76.6131	30	8
BL2	BALTIMORE	MD	39.2367	76.5844	30	8
BL3	BALTIMORE	MD	39.3147	76.6142	30	8
CKY	COCKEYSVILLE	MD	39.4611	76.6311	30	9
ESX	ESSEX	MD	39.3531	76.4814	31	9
GRN	GREENBELT	MD	39.0200	76.8278	29	7
RVB	RIVIERA BEACH	MD	39.1597	76.5117	30	7
RCK	ROCKVILLE	MD	39.1133	77.1072	28	7
SUT	SUITLAND-SILVER HILL	MD	38.8533	76.9319	29	6
POR	PORTLAND	ME	43.6597	70.2622	55	34
BAY	BAYONNE	NJ	40.6811	74.1197	40	17
CM1	CAMDEN	NJ	39.9231	75.0972	36	12
DUM	DUMONT	NJ	40.9378	73.9950	41	18
ESO	EAST ORANGE	NJ	40.7564	74.2006	40	17
EZ2	ELIZABETH	NJ	40.6411	74.2078	40	16
FLM	FLEMINGTON	NJ	40.5167	74.8100	37	16
LIN	LINDEN	NJ	40.6044	74.2533	39	16
MCG	MC GUIRE AFB	NJ	40.0486	74.5839	38	13
MON	MONMOUTH CO	NJ	40.3278	74.2667	39	14
NWR	NEWARK	NJ	40.7328	74.1781	40	17
NWB	NEW BRUNSWICK	NJ	40.4822	74.4408	39	15
PLN	PLAINFIELD	NJ	40.6011	74.4419	39	16
VIN	VINELAND	NJ	39.4922	75.0208	36	9
HM2	HEMPSTEAD	NY	40.8917	73.5986	42	18
NY2	NEW YORK CITY	NY	40.7358	73.8169	41	17
NY5	NEW YORK CITY	NY	40.7394	73.9861	41	17
N10	NEW YORK CITY	NY	40.5972	74.1264	40	16
N11	NEW YORK CITY	NY	40.7775	73.9086	41	17
N12	NEW YORK CITY	NY	40.6719	73.9778	41	17
WNS	WINDSOR, ONT	ON	42.3160	83.0434	4	26
SR2	SARNIA, ONT	ON	42.9785	82.4054	7	30
CR3	CORUNNA, ONT	ON	42.9130	82.4529	7	30
LND	LONDON, ONT	ON	42.9896	81.2232	12	30
SMC	SIMCOE, ONT	ON	42.8560	80.2693	15	30
NAN	NANTICOKE, ONT	ON	42.8749	79.9948	17	30
KCH	KITCHENER, ONT	ON	43.4578	80.4722	15	33
STC	ST. CATHERINES, ONT	ON	43.1654	79.2397	20	31
HL1	HAMILTON, ONT	ON	43.2826	79.7872	17	32
HML	HAMILTON, ONT	ON	43.2586	79.8432	17	32
TR1	TORONTO, ONT	ON	43.6601	79.3878	19	34
TR2	TORONTO, ONT	ON	43.6472	79.3671	19	34
SCR	SCARBOROUGH, ONT	ON	43.7485	79.2749	19	35

TABLE 6.1. (continued)

I.D.	Location	State	Lat.	Lon.	ROM Grid Cell	
			(deg.,N)	(deg.,W)	x	y
NYK	NORTH YORK, ONT	ON	43.7197	79.3390	19	35
NK1	NORTH YORK, ONT	ON	43.7358	79.4366	19	35
EB1	ETOBICOKE, ONT	ON	43.6501	79.5840	18	34
EB2	ETOBICOKE, ONT	ON	43.6169	79.5228	18	34
BLG	BURLINGTON, ONT	ON	43.3158	79.8014	17	32
OK2	OAKVILLE, ONT	ON	43.4174	79.6993	18	33
OSH	OSHAWA, ONT	ON	43.8962	78.8535	21	36
MSG	MISSISSAUGA, ONT	ON	43.5703	79.6106	18	34
AG1	ALLEGHENY CO	PA	40.3819	80.1856	16	15
AG3	ALLEGHENY CO	PA	40.4428	79.9881	17	15
PT2	PITTSBURGH	PA	40.4656	79.9611	17	15
PT3	PITTSBURGH	PA	40.4367	79.9547	17	15
PWM	PRINCE WILLIAM CO	VA	38.6419	77.5283	26	4
CHS	CHARLESTON	WV	38.3419	81.6200	10	3

TABLE 6.2. NO2 MONITORING STATIONS - NEROS REGION - 1980

I.D.	Location	State	Lat. (deg.,N)	Lon. (deg.,W)	ROM Grid x	Cell y
HF2	HARTFORD	CT	41.7608	72.6789	46	23
DC1	WASHINGTON	DC	38.9036	77.0517	28	6
DC2	WASHINGTON	DC	38.9753	77.0228	28	6
NC1	NEW CASTLE CO	DE	39.8083	75.4500	35	11
WIL	WILMINGTON	DE	39.7333	75.5500	34	11
AS1	ASHLAND	KY	38.4436	82.6131	6	3
BS1	BOSTON	MA	42.3483	71.0992	52	27
BS3	BOSTON	MA	42.3781	71.0283	52	27
WAT	WATERTOWN	MA	42.3747	71.1825	52	27
WO1	WORCESTER	MA	42.2586	71.8006	49	26
AA4	ANNE ARUNDEL CO	MD	39.1014	76.7278	30	7
BL1	BALTIMORE	MD	39.2997	76.6131	30	8
BL2	BALTIMORE	MD	39.2367	76.5844	30	8
BL3	BALTIMORE	MD	39.3147	76.6142	30	8
BL7	BALTIMORE CO	MD	39.5150	76.4311	31	10
CKY	COCKEYSVILLE	MD	39.4611	76.6311	30	9
ESX	ESSEX	MD	39.3531	76.4814	31	9
GRN	GREENBELT	MD	39.0200	76.8278	29	7
HRF	HARFORD CO	MD	39.6269	76.3294	31	10
RVB	RIVIERA BEACH	MD	39.1597	76.5117	30	7
RCK	ROCKVILLE	MD	39.1133	77.1072	28	7
SUT	SUITLAND-SILVER HILL	MD	38.8533	76.9319	29	6
DT2	DETROIT	MI	42.3583	83.0975	4	27
DT3	DETROIT	MI	42.4333	83.0036	4	27
DT4	DETROIT	MI	42.3339	83.0333	4	27
BAY	BAYONNE	NJ	40.6811	74.1197	40	17
CM1	CAMDEN	NJ	39.9231	75.0972	36	12
DUM	DUMONT	NJ	40.9378	73.9950	41	18
ESO	EAST ORANGE	NJ	40.7564	74.2006	40	17
EZ2	ELIZABETH	NJ	40.6411	74.2078	40	16
FLM	FLEMINGTON	NJ	40.5167	74.8100	37	16
MCG	MC GUIRE AFB	NJ	40.0486	74.5839	38	13
NWR	NEWARK	NJ	40.7328	74.1781	40	17
NWB	NEW BRUNSWICK	NJ	40.4822	74.4408	39	15
PSB	PHILLIPSBURG	NJ	40.6833	75.1869	36	17
PLN	PLAINFIELD	NJ	40.6011	74.4419	39	16
VIN	VINELAND	NJ	39.4922	75.0208	36	9
BF1	BUFFALO	NY	42.8781	78.8094	21	30
HM1	HEMPSTEAD	NY	40.7453	73.5869	42	17
NY2	NEW YORK CITY	NY	40.7358	73.8169	41	17
NY5	NEW YORK CITY	NY	40.7394	73.9861	41	17
N10	NEW YORK CITY	NY	40.5972	74.1264	40	16
N11	NEW YORK CITY	NY	40.7775	73.9086	41	17
N12	NEW YORK CITY	NY	40.6719	73.9778	41	17
SY1	SYRACUSE	NY	43.0453	76.1478	32	31
WPL	WHITE PLAINS	NY	41.0522	73.7642	41	19
AK1	AKRON	OH	41.0764	81.5181	10	19
CAN	CANTON	OH	40.7975	81.3750	11	17
CB1	COLUMBUS	OH	40.0000	83.0417	4	13
DA1	DAYTON	OH	39.7692	84.2119	1	11
DA4	DAYTON	OH	39.7592	84.2000	1	11

TABLE 6.2. (continued)

I.D.	Location	State	Lat. (deg.,N)	Lon. (deg.,W)	ROM Grid x	Cell y
DA5	DAYTON	OH	39.7814	84.2014	1	11
STU	STEUBENVILLE	OH	40.3594	80.6231	14	15
YG2	YOUNGSTOWN	OH	41.0997	80.6503	14	19
WNS	WINDSOR, ONT	ON	42.3160	83.0434	4	26
SR2	SARNIA, ONT	ON	42.9785	82.4054	7	30
CR3	CORUNNA, ONT	ON	42.9130	82.4529	7	30
LND	LONDON, ONT	ON	42.9896	81.2232	12	30
SMC	SIMCOE, ONT	ON	42.8560	80.2693	15	30
NAN	NANTICOKE, ONT	ON	42.8749	79.9948	17	30
KCH	KITCHENER, ONT	ON	43.4578	80.4722	15	33
STC	ST. CATHERINES, ONT	ON	43.1654	79.2397	20	31
HL1	HAMILTON, ONT	ON	43.2826	79.7872	17	32
HML	HAMILTON, ONT	ON	43.2586	79.8432	17	32
TR1	TORONTO, ONT	ON	43.6601	79.3878	19	34
TR2	TORONTO, ONT	ON	43.6472	79.3671	19	34
SCR	SCARBOROUGH, ONT	ON	43.7485	79.2749	19	35
NYK	NORTH YORK, ONT	ON	43.7197	79.3390	19	35
NK1	NORTH YORK, ONT	ON	43.7358	79.4366	19	35
EB1	ETOBICOKE, ONT	ON	43.6501	79.5840	18	34
EB2	ETOBICOKE, ONT	ON	43.6169	79.5228	18	34
BLG	BURLINGTON, ONT	ON	43.3158	79.8014	17	32
OK2	OAKVILLE, ONT	ON	43.4174	79.6993	18	33
OSH	OSHAWA, ONT	ON	43.8962	78.8535	21	36
MSG	MISSISSAUGA, ONT	ON	43.5703	79.6106	18	34
AG3	ALLEGHENY CO	PA	40.4428	79.9881	17	15
ALN	ALLENTOWN	PA	40.6186	75.4489	35	16
BAD	BADEN	PA	40.6356	80.2308	16	16
BVF	BEAVER FALLS	PA	40.7478	80.3167	15	17
BET	BETHLEHEM	PA	40.6203	75.3644	35	16
BRI	BRISTOL (BOROUGH)	PA	40.2475	74.9972	37	14
CHL	CHARLEROI	PA	40.1469	79.9033	17	13
CHT	CHESTER	PA	39.8369	75.3747	35	12
ERE	ERIE	PA	42.1394	80.0467	16	25
HAR	HARRISBURG	PA	40.2444	76.8472	29	14
JNS	JOHNSTOWN	PA	40.3097	78.9158	21	14
KUT	KUTZTOWN	PA	40.5108	75.7853	33	16
LAN	LANCASTER CITY	PA	40.0439	76.2867	31	13
NCL	NEW CASTLE	PA	40.9958	80.3467	15	18
NRS	NORRISTOWN	PA	40.1122	75.3106	35	13
PH1	PHILADELPHIA	PA	40.0089	75.0983	36	13
PH7	PHILADELPHIA	PA	40.0764	75.0119	36	13
PH8	PHILADELPHIA	PA	39.9467	75.1639	36	12
P10	PHILADELPHIA	PA	39.9572	75.1731	36	12
PT2	PITTSBURGH	PA	40.4656	79.9611	17	15
PT3	PITTSBURGH	PA	40.4367	79.9547	17	15
RDG	READING	PA	40.3208	75.9278	33	14
SC1	SCRANTON	PA	41.4431	75.6244	34	21
WLK	WILKES-BARRE	PA	41.2378	75.8958	33	20
YOR	YORK	PA	39.9656	76.6992	30	12
PV1	PROVIDENCE	RI	41.8208	71.4081	51	23
ARL	ARLINGTON CO	VA	38.8575	77.0592	28	6

TABLE 6.2. (continued)

I.D.	Location	State	Lat.	Lon.	ROM Grid Cell	
			(deg.,N)	(deg.,W)	x	y
FX3	FAIRFAX CO	VA	38.7422	77.0775	28	5
MCL	MC LEAN	VA	38.9344	77.1983	28	6
PWM	PRINCE WILLIAM CO	VA	38.6419	77.5283	26	4
SVC	SEVEN CORNERS	VA	38.8678	77.1431	28	6
CHS	CHARLESTON	WV	38.3419	81.6200	10	3

follows describes how a subset of the available data was used in an aggregated sense for comparison with ROM results.

6.1.2 Data Aggregation

The performance of the ROM for predicting NO_x and NO_2 concentrations must be tested against observed data having a clear, strong "signal" for these species. In other words, the ambient concentrations should be at sufficiently high levels over large areas (on the order of ROM grid cells) and over several-hour time periods. Frequently, ambient concentrations of NO_x and NO_2 are below the detectable limits of most monitors deployed in the field, ≈ 5 ppb. This is especially true in non-urban areas. The ROM should be able to model non-urban, regional concentrations of NO_x and NO_2 . The problem here, however, is obtaining credible estimates of these concentrations when they are in the noise level of most monitors. In an effort to circumvent these problems for the surface analysis discussed here, data from NO_x and NO_2 monitors were aggregated in individual urban areas with large NO_x source emissions. These were major metropolitan areas that contained multiple monitoring stations.

Table 6.3 lists the urban areas considered in the analyses and identifies the monitoring stations whose data were aggregated for each area. The number of monitors in each group varied from 2 for the Boston and Washington areas to 10 for the New York area. Observed data values less than 5 ppb were considered as missing values since they are within the noise range of the monitors. The observed data were then passed through the same high-frequency filter used for O_3 , to eliminate frequencies in the data that are beyond the ROM's ability to simulate with the current grid resolution.

Figure 6.3 shows the effect of the filter on the NO_x data record for a Baltimore station during the simulation period. As expected, the data show considerable hour to hour variations, although a mid-morning peak is usually discernable, corresponding to the heavier NO_x emissions associated with the morning traffic period, and a late evening secondary maximum often occurs as the surface layer stability increases at night. Surprisingly, the effect of the filter is not as pronounced as might be expected given the temporal variability of the NO_x concentrations. The sharp peaks in the data record have been dampened to a degree, but overall the filter's effect is similar to that seen on the O_3 record.

For each urban area the predicted data set was prepared by aggregating hour-averaged layer 1 ROM predictions from each of the grid cells containing relatively high emissions within and surrounding the urban area. Table 6.4 lists the (x, y) coordinates of the ROM grid cells involved for each of the urban areas. The ROM explicitly predicts NO_2 but does not explicitly predict NO_x . The NO_x predictions

TABLE 6.3. STATIONS INCLUDED IN AGGREGATE GROUPS FOR
NO_x and NO₂ ANALYSIS

Urban Area Station Group	Station ID's in NO _x Group	Station ID's in NO ₂ Group
Baltimore	BL1, BL2, BL3, RVB	BL1, BL2, BL3, RVB
Boston	BS3, SOM	BS1, WAT
Detroit	-	DT2, DT3, DT4, WNS
New York City	BAY, DUM, ESO, EZ2, LIN, N10, N11, N12, NY2, NY5, PLN	BAY, DUM, ESO, EZ2, HM1, N10, N11, N12, NY2, NY5, PLN
Philadelphia	-	CM1, NRS, P10, PH1, PH7, PH8
Pittsburgh	AG1, AG3, PT2, PT3	AG3, PT2, PT3
Toronto	EB1, EB2, MSG, NK1, NYK, SCR, TR1, TR2	EB1, EB2, MSG, NK1, NYK, SCR, TR1, TR2
Washington	DC1, SUT	ARL, DC1, FX3, MCL, SUT, SVC

TABLE 6.4. ROM GRID CELLS INCLUDED IN AGGREGATE GROUPS FOR
NO_x and NO₂ ANALYSIS

Urban Area Grid Cell Group	Grid Cells in NO _x Group (x, y)	Grid Cells in NO ₂ Group (x, y)
Baltimore	(30, 7), (30, 8), (30, 9)	(30, 7), (30, 8), (30, 9)
Boston	(52,26), (52,27)	(52,26), (52,27)
Detroit	-	(3,26), (3,27), (4,25), (4,26), (4,27)
New York City	(39,16), (39,17), (40,16), (40,17), (40,18), (41,16), (41,17), (41,18), (42,16), (42,17)	(39,16), (39,17), (40,16), (40,17), (40,18), (41,16), (41,17), (41,18), (42,16), (42,17)
Philadelphia	-	(35,12), (35,13), (36,12), (36,13), (37,13)
Pittsburgh	(16,15), (16,16), (17,15), (17,16)	(16,15), (16,16), (17,15), (17,16)
Toronto	(18,34), (18,35), (19,34), (19,35)	(18,34), (18,35), (19,34), (19,35)
Washington	(28, 6), (29, 6)	(28, 5), (28, 6), (29, 6)

were calculated by summing the concentrations of the species that the ROM *does* predict which are detected by the NO_x monitors:

$$NO_x = NO + NO_2 + PAN + HONO + N_2O_5 + NO_3 + \frac{HNO_3}{2.0}$$

Typically, only a fraction of the HNO₃ concentration is detected since there are losses in the sampling line. A nominal value of 50% has been used here for the HNO₃ component of the NO_x measurement (Lonneman, 1988).

Figure 6.4 is presented here for comparison with the data shown in Figure 6.3. The time series of predicted NO_x concentrations for grid cell (30, 8), encompassing much of the city of Baltimore is shown. These data do not demonstrate the hour to hour variability seen in the observations, but they do show the characteristic twin peaks during a diurnal cycle. The overall concentration levels of the predictions are considerably lower than those in the observations.

The purpose of the surface analysis of NO_x and NO₂ concentrations is not necessarily to evaluate the ROM's performance at predicting these species over the domain; the data base is insufficient for that purpose. Rather, it is an attempt to understand how the model translates high anthropogenic fluxes of these precursor emissions into ambient concentrations on the 18.5 km grid scale, and to understand the relationship between these concentrations and the point measurements taken within the high emissions area. Given the nature of the NO_x and NO₂ measurements it would not be unexpected for the model to show underpredictions. A significant question is whether the degree of systematic variance between these predictions and measurements is constant or variable from location to location. If the relationship appears to be constant, then significant departures may indicate local problems with the emissions inventory.

6.2 RESULTS

6.2.1 Grouped Station Analysis

Plots of the cumulative frequency distributions of observed and predicted concentrations for NO_x and NO₂ for each of the aggregate city groupings were made on the processed data sets for the entire simulation period. The data are presented for both daytime hours only (11 hour period beginning at 0800 h, LST) and for all hours of the day. Figure 6.5 presents the results for NO_x and Figure 6.6 presents the results for NO₂. It is immediately apparent that the ROM has systematically underpredicted the NO_x and NO₂ concentrations for all city groups. There are, however, some interesting variations. The frequency distributions for NO_x show a linear pattern until the 80th to 90th percentiles after which they tend to bend

downward toward increasing underprediction. The distributions for NO_2 are also linear through the 80th to 90th percentiles. Beyond that point, however, they generally bend upward toward decreasing underprediction. The reason for this difference is not immediately obvious. One possible reason for the difference may have to do with the different nature of the source functions under high concentration conditions. The fraction of NO_2 that is photochemically generated compared to the part that comes from direct emissions is relatively larger under high concentration conditions than under low concentration conditions. Since the ROM is expected to perform better for secondary pollutants compared to primary ones because of the subgrid scale gradient problem, we see the performance for NO_2 improving at these upper concentration levels. For NO_x , however, the primary fraction is dominant under all concentration levels, and the subgrid problem becomes only more accentuated under conditions of high concentrations leading to increasing underpredictions.

The general nature of the distributions remains the same whether one considers daytime hours only or all hours. Through approximately the 90th percentile the daytime and all hour distributions are often nearly the same. The greatest difference is seen at the higher concentration levels where the ROM predictions show relatively higher concentrations when the evening and nighttime hours are included. The observations do not change as much by the inclusion of the nighttime hours, implying that some of the highest observed concentrations occur during the daytime period. The ROM's vertical structure at night typically shows a decoupling of the first prognostic model layer above ground, layer 1, from those layers above it, leading to increased stability and potential for a build-up of emissions products in this layer. The predicted concentration profiles reflect this phenomenon. Observed concentration distributions often shift to include higher concentrations during the nighttime hours, but the difference is not as great as that seen in the predictions. The real world may have other factors that mitigate this day-night effect seen in the predicted concentrations.

The NO_x and NO_2 results for the New York aggregate group are perhaps the most statistically significant results presented here. There were more monitoring sites and more grid cells included in this group than for any other, and the distributions for New York follow the general characteristics described above with fewer variations than other groups. The Pittsburgh NO_x data show some anomalous behavior at concentrations above the 95th percentile, and the Toronto NO_2 data show surprising agreement with predictions at higher concentration levels considering the systematic underpredictions among all other groups. This may result from a combination of factors including the increased nighttime stability over adjacent Lake Ontario developed by the model, leading to a heavy build-up of emissions products in the ROM layer 1. Also, Canadian NO_2 concentration data are reported to the nearest 10 ppb, leading to the staircase effect in the frequency distribution.

Table 6.5 presents selected data from the cumulative frequency distributions shown in the previous figures. The concentrations at percentile levels 25, 50, 75, 90, and 100 are given for the NO_x and NO_2 distributions for the daytime data set. Table 6.6 presents a similar data set, except for all hours of the simulation. The ratio of observed to predicted concentrations at the selected points of the frequency distributions generally varies between 1.5 and 3.0, with ratios outside of this range standing more or less as outliers. Table 6.7 presents a summary of the observed/predicted concentration ratios averaged over all station groups for the 50th and the 90th percentiles of the cumulative frequency distribution.

TABLE 6.7. AVERAGE RATIO (OBS./PRED.) OVER STATION GROUPS AT 50TH AND 90TH PERCENTILES OF CUMULATIVE FREQUENCY DISTRIBUTIONS

	Daytime 08-19h, LST		All hours	
	Percentile 50 th	Percentile 90 th	Percentile 50 th	Percentile 90 th
NO_x	1.8	2.3	1.9	2.5
NO_2	2.2	2.2	2.1	1.9

From these data it is clear that the ROM is underpredicting both NO_x and NO_2 significantly. The problem may lie partially in the non-regional character of the monitoring site locations and partially in the amounts of precursor material in the emissions inventory. The absence of surface predictions (ROM layer 0) for NO_x may be significant here. There may also be an inherent limitation in the ROM's ability to predict primary species from distributed emissions sources because of the coarse grid resolution. In any case the results appear to be consistent from city to city for the analysis done here. There is some indication based on relatively higher ratios in the analysis for the Baltimore-Washington combined area that the emissions inventory is more deficient in NO_x in that area than it is in the other cities studied. In general however, the apparent underprediction of NO_x and NO_2 point measurements has not seriously affected the ROM's ability to predict regional O_3 concentrations.

6.2.2 Spatial Pattern Analysis

Although considerably fewer monitoring stations were available for NO_2 and NO_x measurements during the summer of 1980 than were available for O_3 , a limited analysis of spatial patterns is attempted here. Another obstacle encountered in this spatial pattern analysis was the data sparsity in many areas of the grid and the local

TABLE 6.5. CONCENTRATIONS (ppb) OF OBSERVED AND PREDICTED NO_x AND NO₂ AT SELECTED PERCENTILES OF THE CUMULATIVE FREQUENCY DISTRIBUTIONS FOR SELECTED SOURCE AREAS; DAYLIGHT HOURS ONLY (08-19h, LST) OF SIMULATION PERIOD (80196-80244).

		PERCENTILES				
		25	50	75	90	100
<u>Baltimore</u>						
NO ₂	obs.	11.0	20.0	33.0	48.0	102.0
	pred.	6.8	9.3	13.6	19.0	42.4
	(obs./pred.)	(1.6)	(2.1)	(2.4)	(2.5)	(2.4)

NO _x	obs.	14.0	26.0	48.0	70.0	401.0
	pred.	9.5	13.3	18.9	26.5	66.4
	(obs./pred.)	(1.5)	(2.0)	(2.5)	(2.6)	(6.0)
<u>Boston</u>						
NO ₂	obs.	13.0	28.0	51.0	73.0	119.0
	pred.	9.0	12.2	18.3	24.7	47.5
	(obs./pred.)	(1.4)	(2.3)	(2.8)	(3.0)	(2.5)

NO _x	obs.	12.0	25.0	41.0	69.0	330.0
	pred.	14.7	19.7	27.4	37.8	69.0
	(obs./pred.)	(0.81)	(1.3)	(1.5)	(1.8)	(4.8)
<u>Detroit</u>						
NO ₂	obs.	14.0	25.0	40.0	54.0	107.0
	pred.	8.4	12.0	18.3	27.2	63.9
	(obs./pred.)	(1.7)	(2.1)	(2.2)	(2.0)	(1.7)
<u>New York</u>						
NO ₂	obs.	15.0	27.0	44.0	62.0	127.0
	pred.	8.5	13.2	21.2	30.0	81.9
	(obs./pred.)	(1.8)	(2.1)	(2.1)	(2.1)	(1.6)

NO _x	obs.	16.0	32.0	57.0	90.0	368.0
	pred.	12.8	19.2	29.9	42.0	121.8
	(obs./pred.)	(1.2)	(1.7)	(1.9)	(2.1)	(3.0)

TABLE 6.5. (Continued)

Philadelphia

NO ₂	obs.	18.0	30.0	45.0	60.0	152.0
	pred.	8.1	12.2	17.9	26.1	65.2
	(obs./pred.)	(2.2)	(2.5)	(2.5)	(2.3)	(2.3)

Pittsburgh

NO ₂	obs.	15.0	23.0	31.0	45.0	169.0
	pred.	7.4	10.4	15.7	23.5	54.9
	(obs./pred.)	(2.0)	(2.2)	(2.0)	(1.9)	(3.1)

NO _x	obs.	12.0	24.0	39.0	67.0	295.0
	pred.	10.5	14.7	21.6	31.9	117.6
	(obs./pred.)	(1.1)	(1.6)	(1.8)	(2.1)	(2.5)

Toronto

NO ₂	obs.	19.0	29.0	40.0	50.0	118.0
	pred.	9.6	15.4	24.5	34.7	74.4
	(obs./pred.)	(2.0)	(1.9)	(1.6)	(1.4)	(1.6)

NO _x	obs.	20.0	40.0	67.0	118.0	492.0
	pred.	12.5	20.9	34.4	51.9	140.7
	(obs./pred.)	(1.6)	(1.9)	(1.9)	(2.3)	(3.5)

Washington, D.C.

NO ₂	obs.	11.0	19.0	32.0	47.0	94.0
	pred.	6.7	9.0	13.2	17.6	45.7
	(obs./pred.)	(1.6)	(2.1)	(2.4)	(2.7)	(2.1)

NO _x	obs.	19.0	31.0	52.0	78.0	275.0
	pred.	11.9	15.7	21.5	27.1	85.7
	(obs./pred.)	(1.6)	(2.0)	(2.4)	(2.9)	(3.2)

TABLE 6.6. CONCENTRATIONS (ppb) OF OBSERVED AND PREDICTED NO_x AND NO₂ AT SELECTED PERCENTILES OF THE CUMULATIVE FREQUENCY DISTRIBUTIONS FOR SELECTED SOURCE AREAS; ALL HOURS OF SIMULATION PERIOD (80196 - 80244).

		PERCENTILES				
		25	50	75	90	100
<u>Baltimore</u>						
NO ₂	obs.	15.0	26.0	40.0	53.0	118.0
	pred.	8.4	12.1	17.3	22.6	78.6
	(obs./pred.)	(1.8)	(2.2)	(2.3)	(2.3)	(1.5)
NO _x	obs.	18.0	35.0	56.0	84.0	401.0
	pred.	11.1	15.4	21.7	28.9	105.0
	(obs./pred.)	(1.6)	(2.3)	(2.6)	(2.9)	(3.8)
<u>Boston</u>						
NO ₂	obs.	16.0	28.0	48.0	67.0	119.0
	pred.	8.2	11.4	16.7	23.8	71.2
	(obs./pred.)	(1.9)	(2.5)	(2.9)	(2.8)	(1.7)
NO _x	obs.	13.0	27.0	49.0	81.0	283.0
	pred.	11.8	16.5	24.0	34.6	148.5
	(obs./pred.)	(1.1)	(1.6)	(2.0)	(2.3)	(1.9)
<u>Detroit</u>						
NO ₂	obs.	16.0	27.0	40.0	54.0	123.0
	pred.	9.4	13.7	20.2	29.1	76.2
	(obs./pred.)	(1.7)	(2.0)	(2.0)	(1.9)	(1.6)
<u>New York</u>						
NO ₂	obs.	18.0	31.0	48.0	66.0	127.0
	pred.	8.5	13.1	20.5	28.9	84.9
	(obs./pred.)	(2.1)	(2.4)	(2.3)	(2.3)	(1.5)
NO _x	obs.	22.0	39.0	66.0	98.0	363.0
	pred.	11.8	17.7	27.0	38.6	174.9
	(obs./pred.)	(1.9)	(2.2)	(2.4)	(2.5)	(2.1)

TABLE 6.6. (Continued)

<u>Philadelphia</u>						
NO ₂	obs.	21.0	34.0	49.0	60.0	152.0
	pred.	9.4	14.1	23.0	36.8	77.1
	(obs./pred.)	(2.2)	(2.4)	(2.1)	(1.6)	(2.0)
<u>Pittsburgh</u>						
NO ₂	obs.	16.0	25.0	35.0	52.0	169.0
	pred.	9.2	14.4	22.0	31.9	72.3
	(obs./pred.)	(1.7)	(1.7)	(1.6)	(1.6)	(2.3)
NO _x	obs.	14.0	26.0	45.0	95.0	295.0
	pred.	12.0	18.4	26.0	37.6	134.1
	(obs./pred.)	(1.2)	(1.4)	(1.7)	(2.5)	(2.2)
<u>Toronto</u>						
NO ₂	obs.	19.0	28.0	40.0	50.0	118.0
	pred.	11.9	20.3	36.3	53.0	99.9
	(obs./pred.)	(1.6)	(1.4)	(1.1)	(0.94)	(1.2)
NO _x	obs.	22.0	40.0	70.0	123.0	492.0
	pred.	13.9	24.7	45.4	73.1	216.4
	(obs./pred.)	(1.6)	(1.6)	(1.5)	(1.7)	(2.3)
<u>Washington, D.C.</u>						
NO ₂	obs.	14.0	23.0	36.0	52.0	114.0
	pred.	8.4	13.0	19.0	26.4	61.1
	(obs./pred.)	(1.7)	(1.8)	(1.9)	(2.0)	(1.9)
NO _x	obs.	21.0	39.0	60.0	102.0	306.0
	pred.	11.6	16.2	22.5	30.6	111.5
	(obs./pred.)	(1.8)	(2.4)	(2.7)	(3.3)	(2.7)

(non-regional) character of the measurements. Most were obtained within urban areas. Nevertheless, we present these data with the stated caveats. The number and distribution of observation sites for NO_x was insufficient to attempt drawing contours; these data are presented on base maps without isopleths connecting them. There were somewhat more stations available for NO_2 , and subjective isopleths were drawn. The uncertainty in these contours, however, is quite high because of the noise in the data.

The analysis considers the average data values during the daily 3-hr period of 0500–0800 h, LST, corresponding to the familiar 6–9 am, LDT statistic used in O_3 precursor analyses of emissions, measurement data, and EKMA (EPA, 1977) isopleths. The spatial analysis was performed for the same episodes discussed in the previous section on O_3 spatial analyses, and the identical model subdomain comprising the Northeast Corridor is used here. Analyses for individual days are shown in Appendix G and the episode-composite results are presented here. Episode composites include the maximum value of the 3-hr average on any day of the given episode. For the observed data set this maximum is determined for each monitoring site and for the predicted data set it is determined for each ROM layer 1 grid cell. Meteorological descriptions of the episodes were given previously.

Episode 1: 80196 - 80199 (July 14 - July 17, 1980)

Figure 6.7 presents the spatial patterns of the episode-maximum daily 3-hr average NO_2 and NO_x concentrations. Figures 6.7(a) and (b) show the observed and predicted fields of NO_2 , respectively, and Figures 6.7(c) and (d) show the observed and predicted fields of NO_x , respectively. The clustering of the observation sites around the major cities is readily apparent in Figures 6.7(a) and (c). The northern NJ-NY metropolitan area and the BW corridor contain most of the monitors. The Philadelphia area has several NO_2 monitors, but only one NO_x monitor. Not surprisingly, the model predictions shown for NO_2 and NO_x also show the highest values over the major city areas of the Northeast Corridor. The highest NO_2 values seen in the New York area in this episode were observed at 60–70 ppb, while the highest predictions were 20–30 ppb. For NO_x , the same concentration range was predicted for NY, but maximum observations were 100–150 ppb. A similar pattern is seen for the other city areas. The larger underprediction for NO_x probably is a result of stronger local source influences on the monitoring sites near the ground for NO_x , especially the NO component during this morning period. The layer-averaged ROM results would tend to diminish this primary source influence compared to near-ground measurements. The ratio of observed to predicted NO_2 values here is similar to that found previously in the grouped station analysis. The spatial patterns outside the cities are difficult to judge from the available monitoring data. The ROM predictions generally show these areas to be less than 10 ppb. The scattered observations are generally higher than the predictions by factors of

2-3, again consistent with the grouped station analysis.

Figures 6.7(b) and (d) show that the Philadelphia area maximum predictions for NO_2 and NO_x are 50 to 100% greater than for the other cities of the Northeast corridor. Observational data are inadequate to substantiate this prediction. It is interesting to note though that the O_3 predictions downwind of Philadelphia for this episode, shown in the last section, are lower than those downwind of other major cities in the Corridor. In light of the NO_x patterns shown here we might speculate that the relatively higher NO_x in the immediate Philadelphia area has suppressed the O_3 there, while the model shows the O_3 generation area far downwind of Philadelphia over the ocean. This pattern is consistent with the higher NO_x concentrations, and presumably, emissions over Philadelphia. Observations of O_3 , however, were indeed high closer in to Philadelphia over central NJ than the ROM would indicate.

Episode 2: 80202 - 80204 (July 20 - July 22, 1980)

The data for this episode are shown in Figure 6.8. The episode-composite maximum 3-hr values of observed and predicted NO_2 are shown in Figures 6.8(a) and (b), respectively, and those for NO_x are shown in Figures 6.8(c) and (d). Results here are very similar to the previous episode. Observations show the highest values near the centers of the metropolitan areas. NO_2 values of 20-30 and 30-40 ppb were predicted over the NY and Philadelphia areas, while the highest observations in the same areas were 60-70 ppb. An isolated NO_x observation of 174 ppb at Hartford, CT appears to be a local anomaly not picked up in the predictions. Relatively higher areas of predicted concentrations appear just north of New York City as well as the city itself, Philadelphia and downwind, the BW Corridor, and Boston. The relatively higher NO_x loading downwind of Philadelphia again seems to have suppressed O_3 levels in the near vicinity and caused delayed O_3 generation in the ROM results.

Episode 3: 80207 - 80209 (July 25 - July 27, 1980)

The observed and predicted NO_2 and NO_x fields for this episode are shown in Figure 6.9. The highest observed values are again in the largest urban areas of the Northeast Corridor. Maximum observed values are generally under 100 ppb for both NO_2 and NO_x . The contoured predicted fields also show maximum value areas over the cities and an extended area over NJ of relatively high values. Maximum predicted values are 20-30 ppb, again lower than the higher observed values by factors of 2 to 3. The highest values predicted over Philadelphia for this episode were lower than those of the previous two episodes, and interestingly, the O_3 values downwind peak over NJ in the ROM predictions instead of over the ocean; i.e., the maximum values have moved closer toward the source of the precursors in the case with lower NO_x concentration values.

Episode 4: 80212 - 80221 (July 30 - August 8, 1980)

Figure 6.10 shows the observed and predicted NO_2 and NO_x patterns for this ten-day episode. Concentrations of NO_2 between 60 and 100 ppb are seen over the urban areas of New York, Philadelphia, and the BW corridor. ROM predictions are in the 20–40 ppb range for the same areas, with the highest concentrations over Philadelphia, 40–50 ppb. Observed NO_x concentrations over New York for the episode were in the 100 to 200 ppb range, with 40–50 ppb predictions in the same area. The highest NO_x predictions were again over Philadelphia, with 60–70 ppb predicted. The O_3 patterns predicted for this episode showed maximum values downwind of NY over Long Island and the ocean as well as over the BW corridor. Maximum predicted O_3 values over central NJ were again depressed compared to observations, similar to the first two episodes described above.

Episode 5: 80238 - 80241 (August 25 - August 28, 1980)

Figure 6.11 presents the observed and predicted patterns of NO_2 and NO_x concentrations for this episode. As discussed in the previous section this episode was meteorologically different than the others in that the surface winds were particularly light and disorganized, with a northeasterly flow along the coast. Sea-breeze influences and potential diurnal flow reversals were more probable during this period. The observed surface concentrations of NO_x over the New York area are particularly interesting. Several stations showed values in the 200–300 ppb range, the highest seen in any of the episodes studied here over an entire metropolitan area. Maximum predicted NO_x values of 40–50 ppb occurred over the NY area during this episode. These were among the highest predicted values for NY, but still considerably less than those observed. The elevated values observed in NY during this period were probably a result of the more complex stability and flow conditions accompanying this episode. The coarseness of the ROM grid and the use of routine meteorological data bases to derive the flow fields does not allow the ROM to adequately describe these particular meteorological phenomena occurring on this urban scale.

The NO_x predictions over the BW corridor and over Boston during this episode were 20–30 ppb, less than over the other urban areas of the East Coast. Comparing these patterns with the maximum predicted O_3 patterns for this episode shown in the previous section, we see that the maximum O_3 concentrations are seen in the near-downwind vicinity of the BW corridor. Maximum values also occur downwind of Boston, and comparable values occur far downwind of New York and Philadelphia, mostly over ocean areas.

In studying the spatial patterns of NO_x and NO_2 over these five episodes several interesting conclusions can be drawn. First, the ROM predicted concentrations over the Northeast Corridor show similar patterns to the observed with the highest values

occurring over major source areas associated, for the most part, with large cities. The highest 0500-0800 h, LST values tend to be underpredicted by the same 2-3 factor seen in the grouped station analysis. The highest predicted concentrations of NO_x and NO_2 , while still considerably less than those observed, are sufficient to slow the chemical processes in the simulation to produce maximum O_3 concentrations considerably farther downwind than those observed. This is due to the reduction of the VOC/NO_x ratio in the presence of increased NO_x which delays the initiation of the period of rapid O_3 production. This phenomenon seems especially pronounced for the Philadelphia area.

The higher NO_x values from Philadelphia ultimately have more potential to produce high O_3 concentrations, but they will be produced farther downstream in time and space because the NMHC/NO_x ratio is low under these circumstances, slowing the chemical processes initially. Observations of O_3 concentrations downwind of Philadelphia show that the central NJ area often had occurrences of high values; certainly more frequently than the ROM predicted. A combination of a large number of uninventoried hydrocarbon emissions (which is thought likely to plague most of the anthropogenic emissions inventory) and an overestimated NO_x emissions source term for the Philadelphia area may be responsible for the problem here. Maximum O_3 concentrations predicted for the NY area were often seen slightly farther downwind than the observations showed them to be, but it is not as obvious in this case that the NO_x concentrations have affected the predicted patterns here as they have for Philadelphia.

The spatial pattern analysis was conducted for the same subdomain as the O_3 spatial analysis so comparisons could be made between the NO_x , NO_2 , and O_3 patterns. This subdomain contained the highest predicted O_3 concentrations and most of the high NO_2 and NO_x concentrations. However the Toronto metropolitan area, outside of this subdomain, consistently generated far higher predicted NO_2 and NO_x concentrations than any other source area. For instance, maximum predicted 3-hr concentrations of NO_x over Toronto during the five episodes studied were in the 100-150 ppb range, while those for New York were in the 40-50 ppb range. The higher atmospheric stability over adjacent Lake Ontario, which fills most of the grid cell in which downtown Toronto is located, may have played a factor in Toronto's higher values. Attendant O_3 concentrations were, however, not greater than those typically seen in the Northeast Corridor.

Finally, the number and location of monitoring stations for NO_2 and NO_x during the summer of 1980 was insufficient to determine spatial patterns over a regional scale with any real confidence. This analysis emphasized the largest urban areas where the majority of the sites were located. For a more meaningful evaluation of spatial patterns of NO_2 and NO_x more stations that are located in regionally representative locations and that are capable of accurately measuring 2-10 ppb concentration values will be necessary.

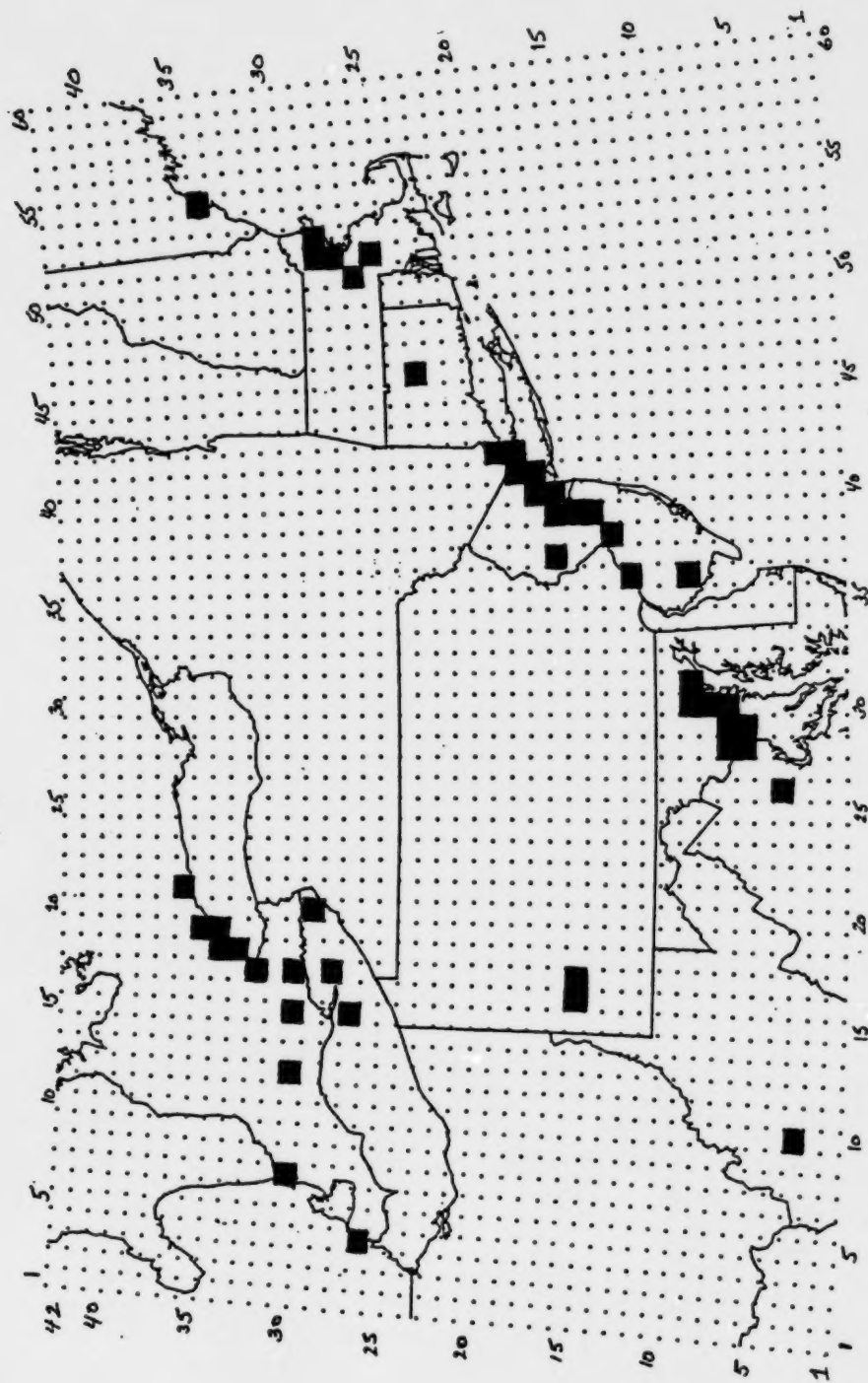


Figure 6.1. ROM grid cells (darkened) containing NO_x monitors.

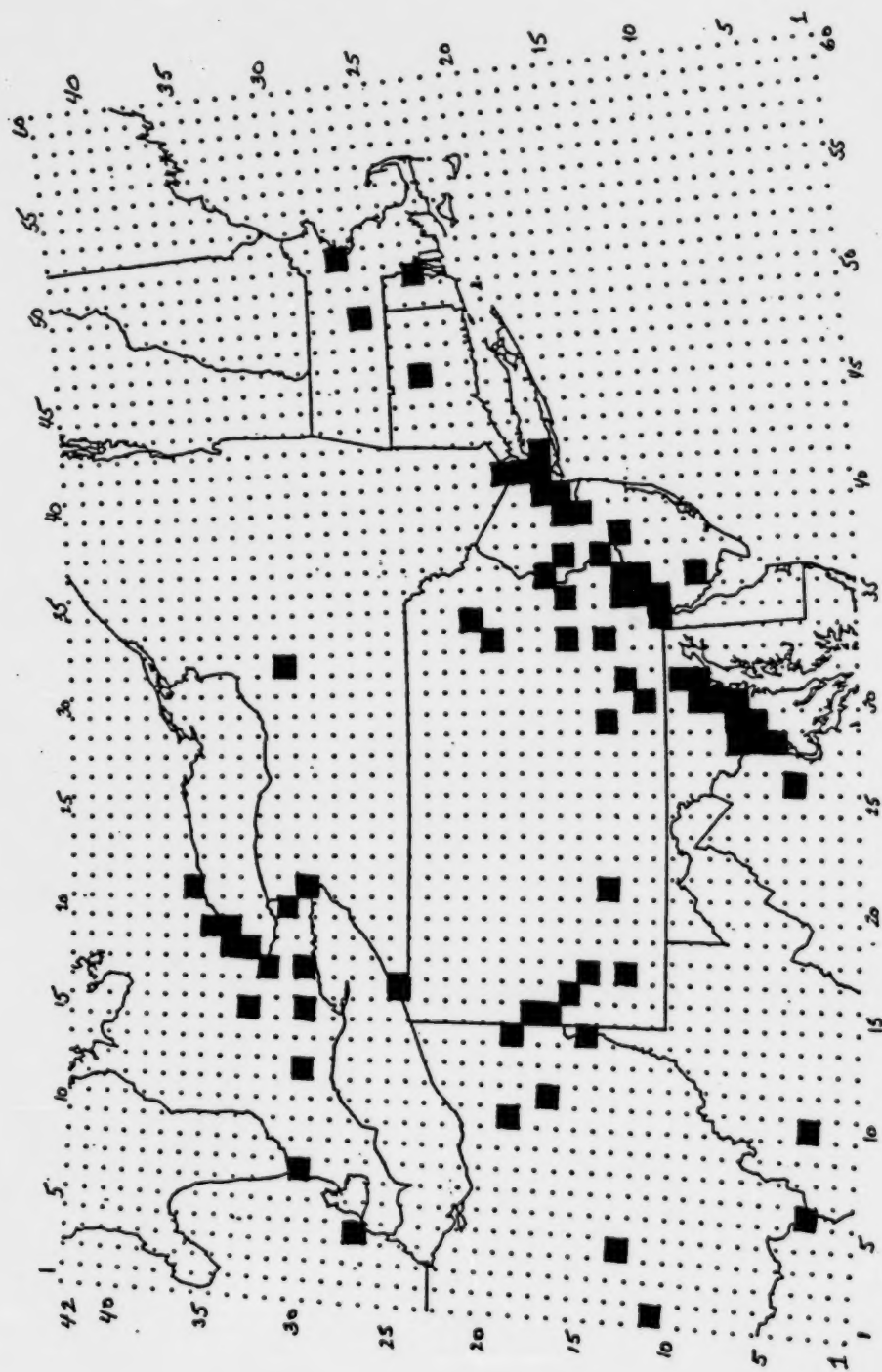


Figure 6.2. ROM grid cells (darkened) containing NO₂ monitors.

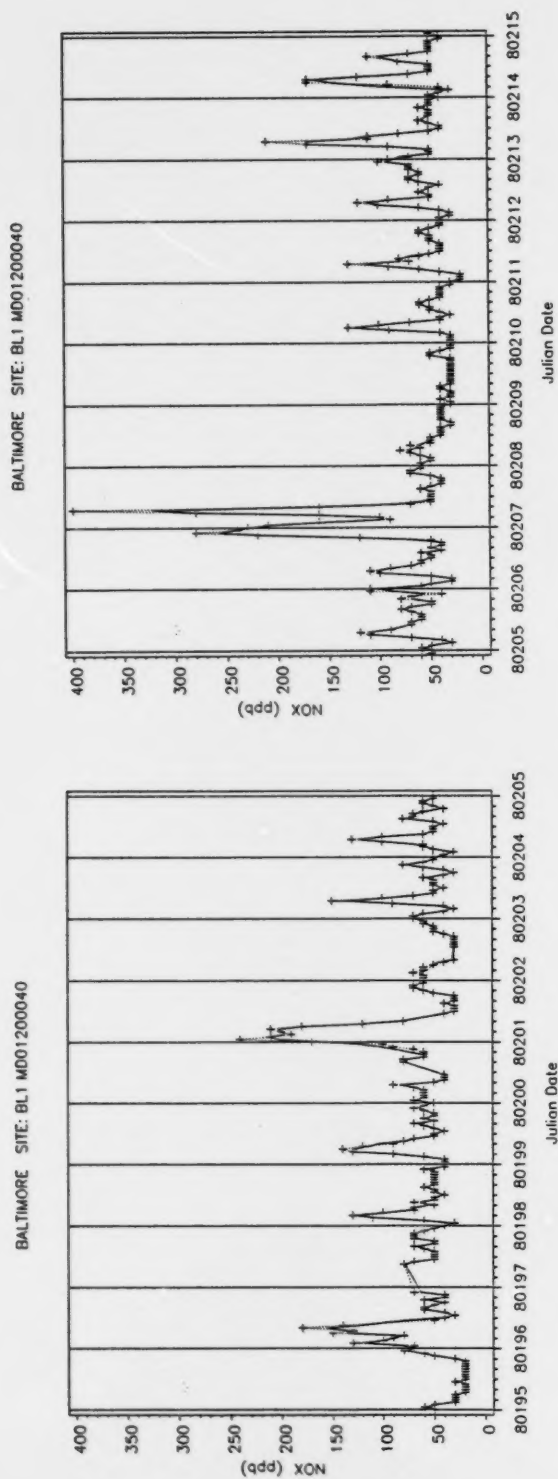
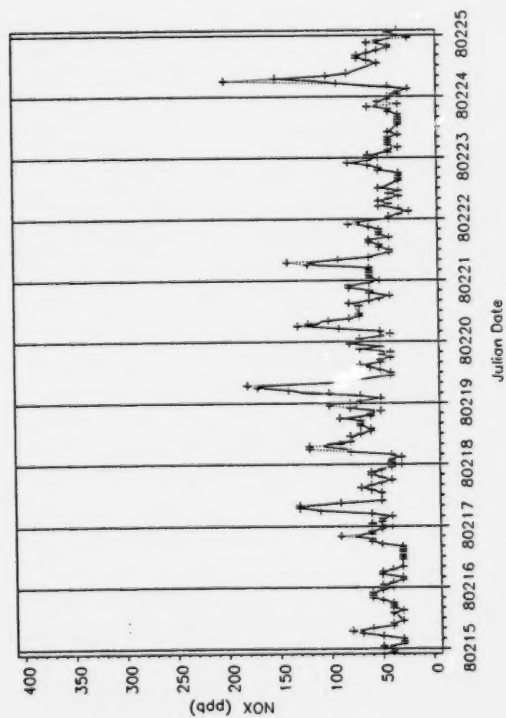
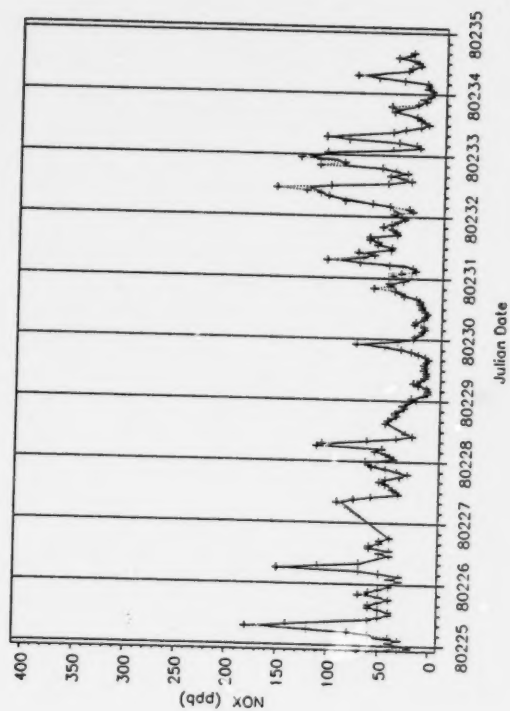


Figure 6.3. Time series, filtered and unfiltered, of BL1 observed NO_x data. The solid line is the filtered data set, and the dotted line is the unfiltered data set.

BALTIMORE SITE: BL1 MD01200040



BALTIMORE SITE: BL1 MD01200040



BALTIMORE SITE: BL1 MD01200040

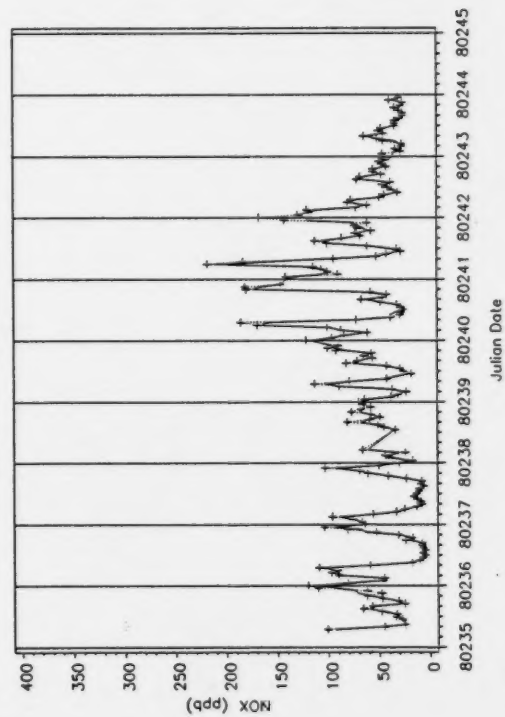
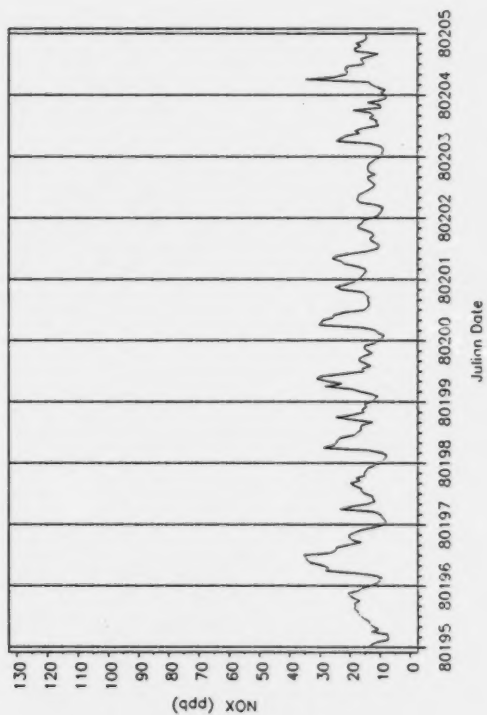


Figure 6.3. (continued)

BALTIMORE COL: 30 ROW: 08
PREDICTED NO_x



BALTIMORE COL: 30 ROW: 08
PREDICTED NO_x

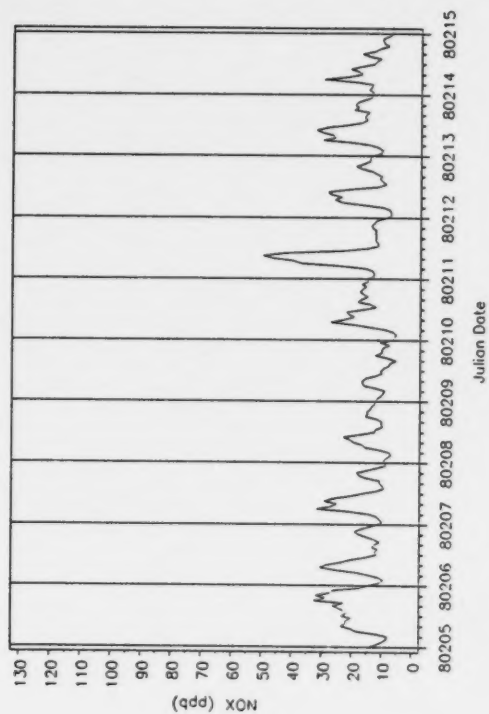
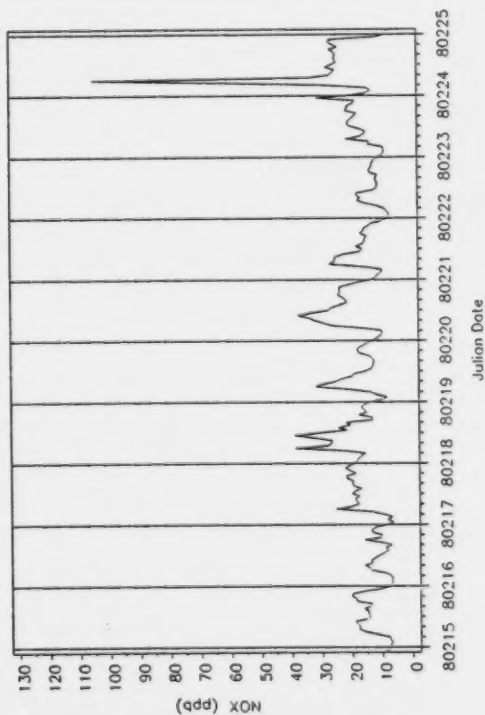
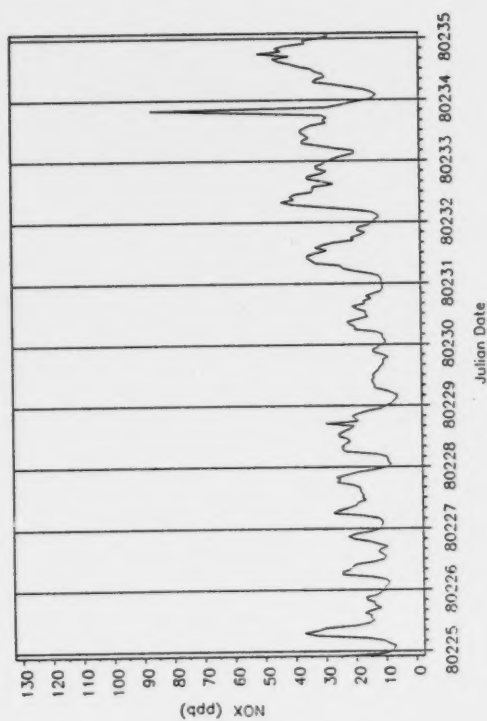


Figure 6.4. Time series of ROM layer 1 NO_x predictions for cell (30, 8), Baltimore area.

BALTIMORE COL: 30 ROW: 08
PREDICTED NOX



BALTIMORE COL: 30 ROW: 08
PREDICTED NOX



BALTIMORE COL: 30 ROW: 08
PREDICTED NOX

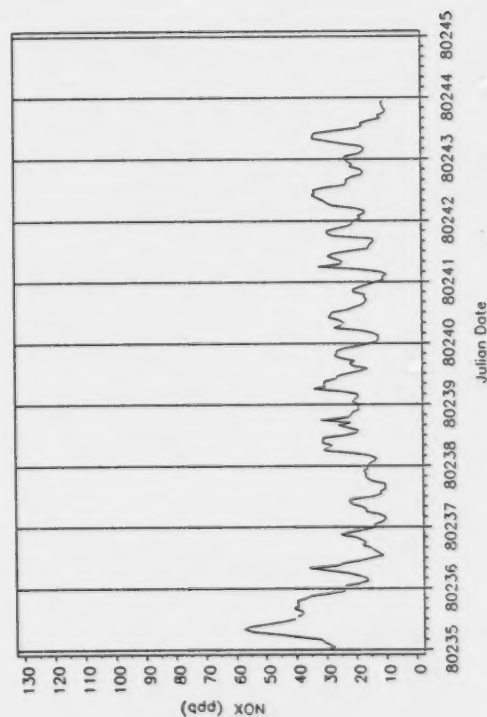


Figure 6.4. (continued)

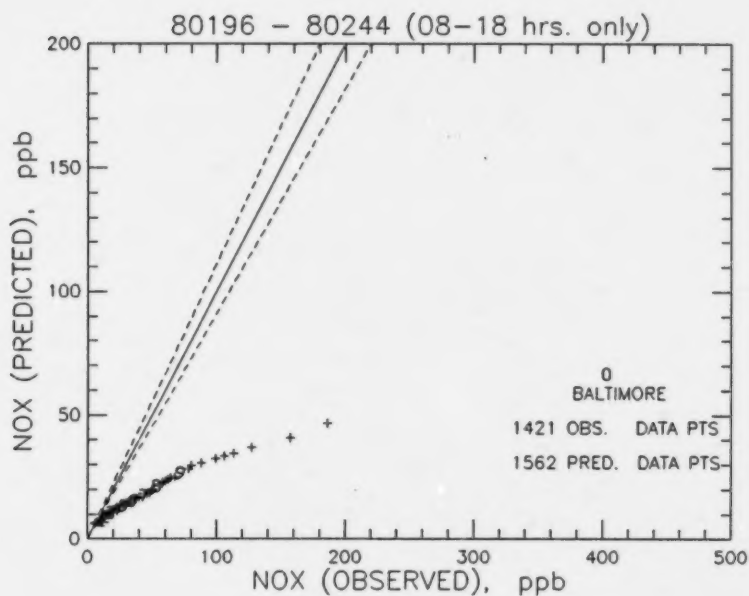
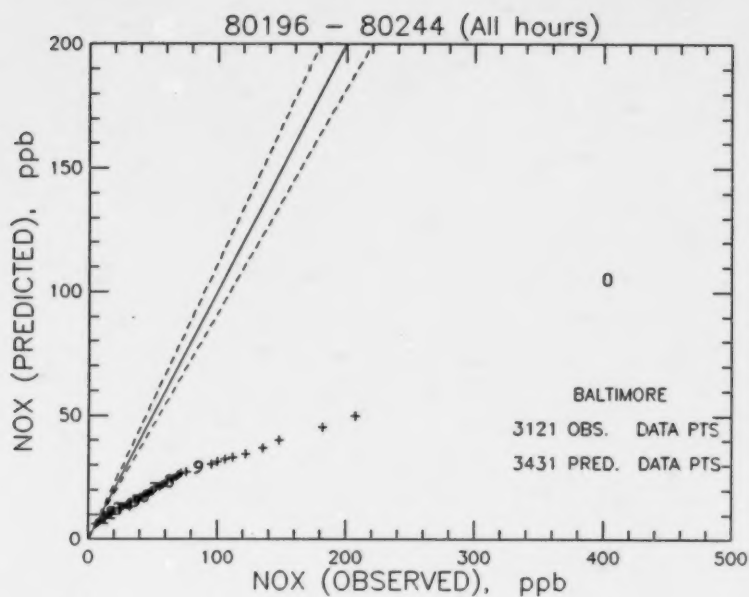


Figure 6.5. Cumulative frequency distributions of observed and predicted NO_x concentrations for selected urban areas over the period July 14–August 30, 1980 for all hours and for daytime hours only. Each percentile level in the distribution is shown and every tenth level is indicated by an integer. The 99.5 percentile is also shown as the rightmost '+' in each figure.

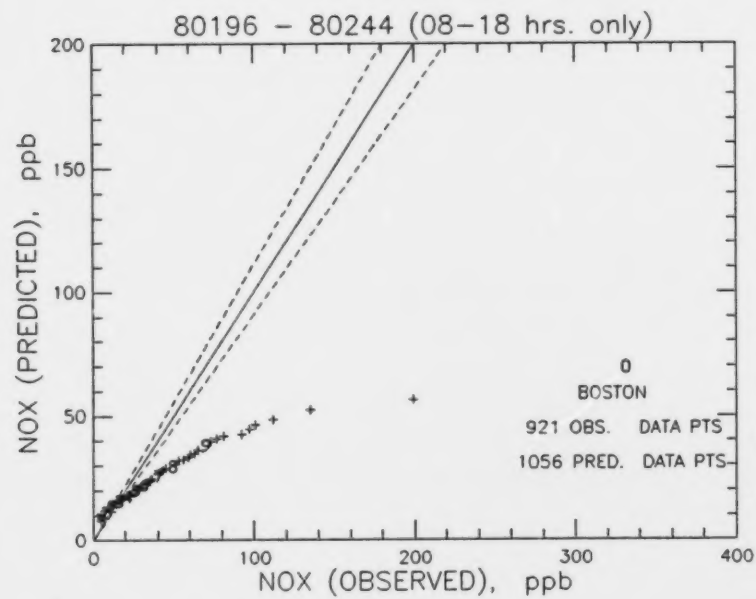
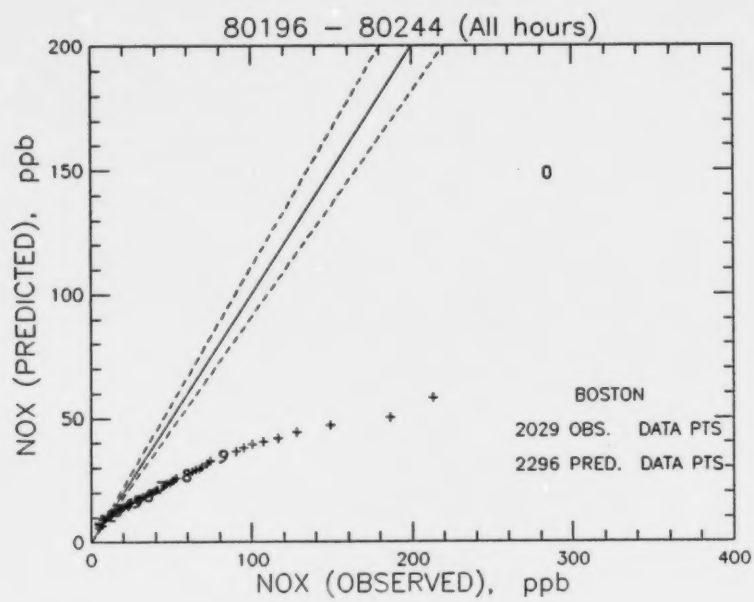


Figure 6.5. (continued)

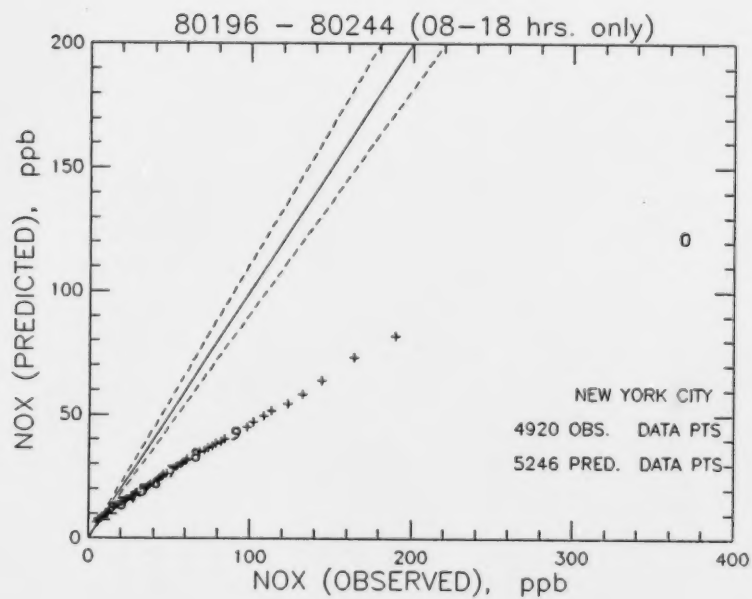
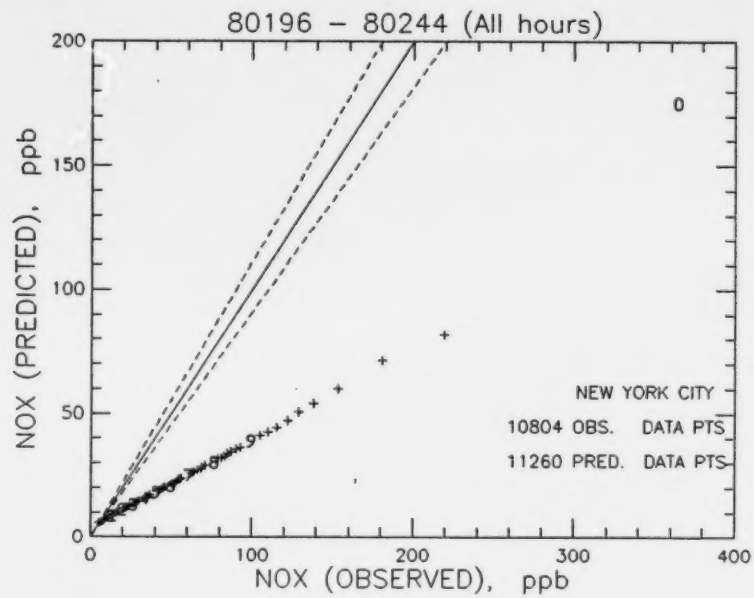


Figure 6.5. (continued)

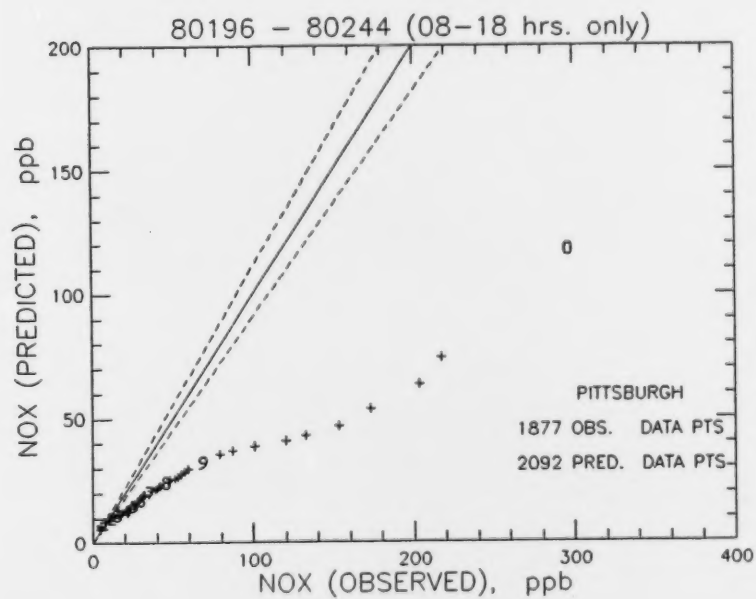
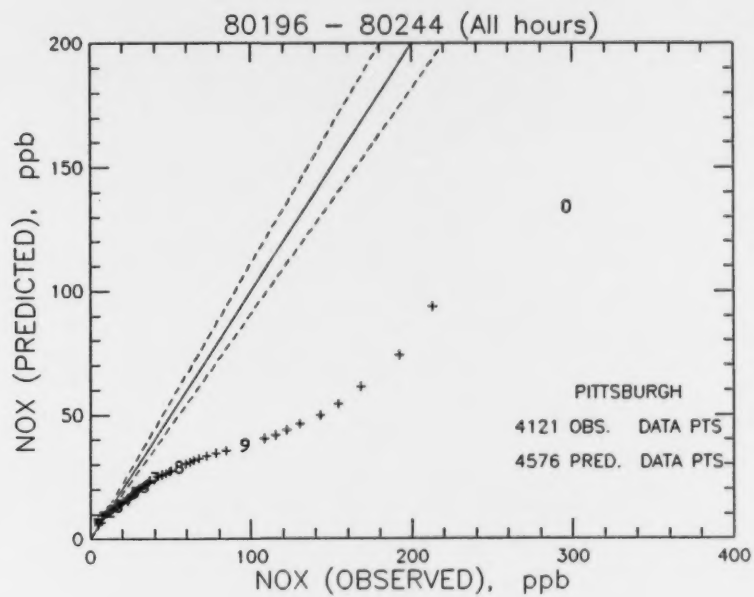


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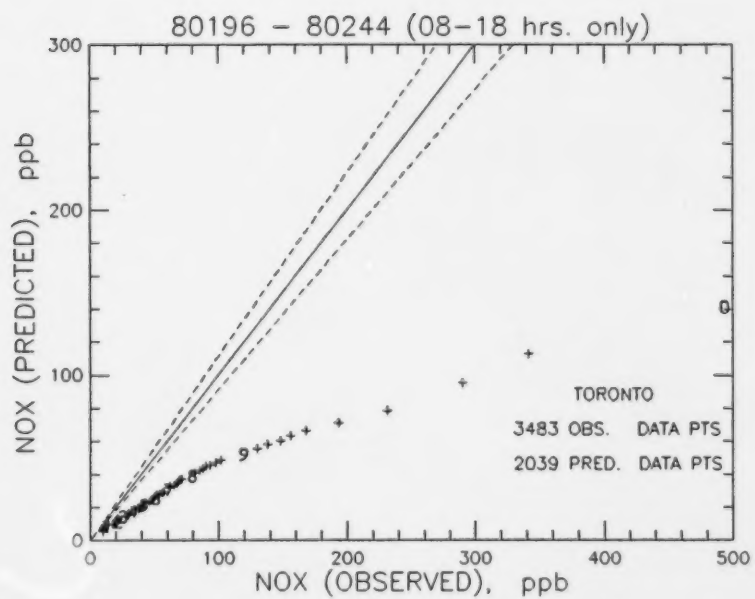
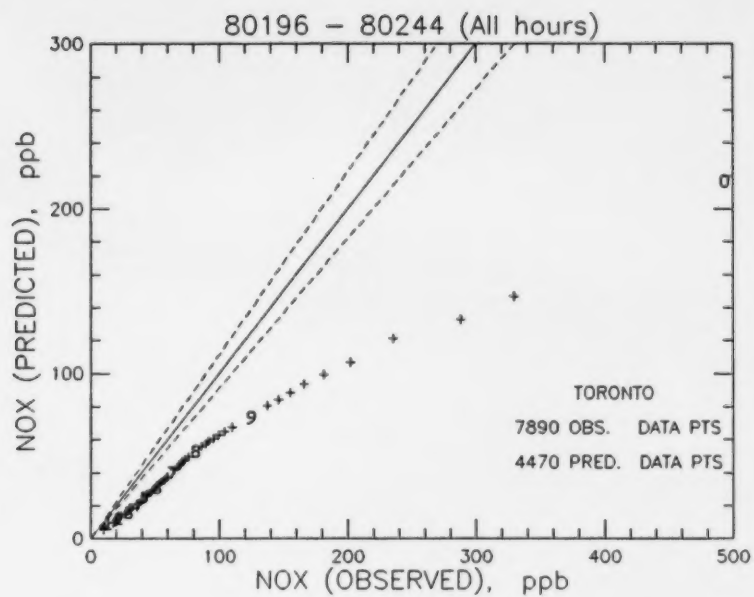


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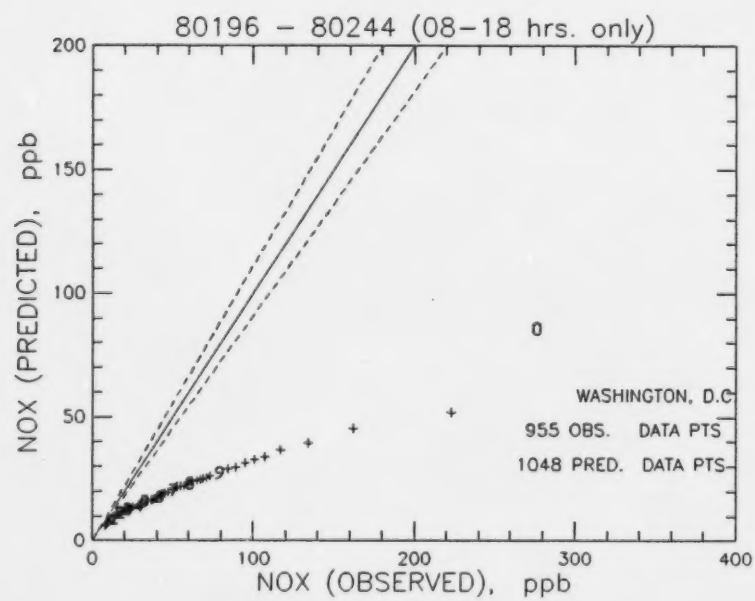
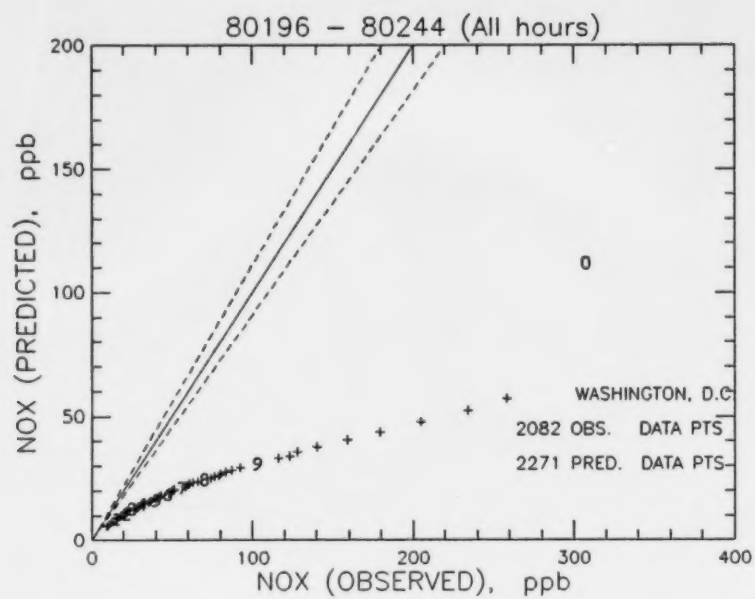


Figure 6.5. (continued)

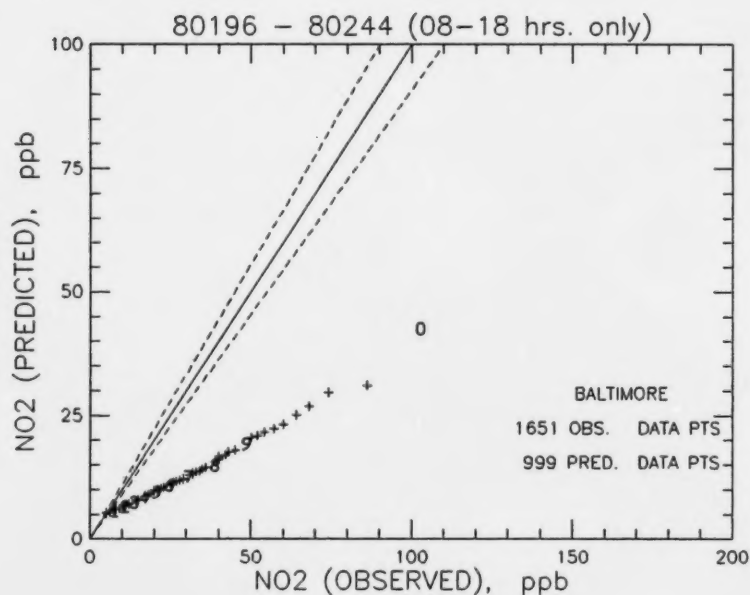
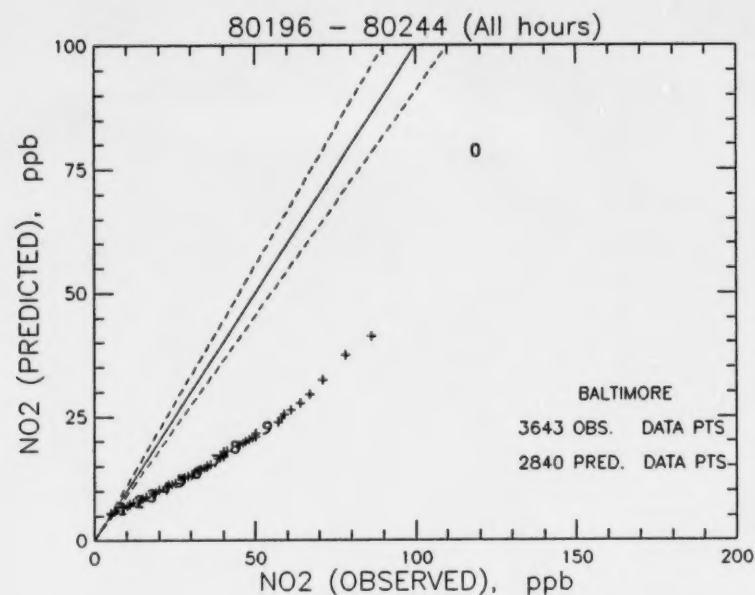


Figure 6.6. Cumulative frequency distributions of observed and predicted NO₂ concentrations for selected urban areas over the period July 14–August 30, 1980 for all hours and for daytime hours only. Each percentile level in the distribution is shown and every tenth level is indicated by an integer. The 99.5 percentile is also shown as the rightmost '+' in each figure.

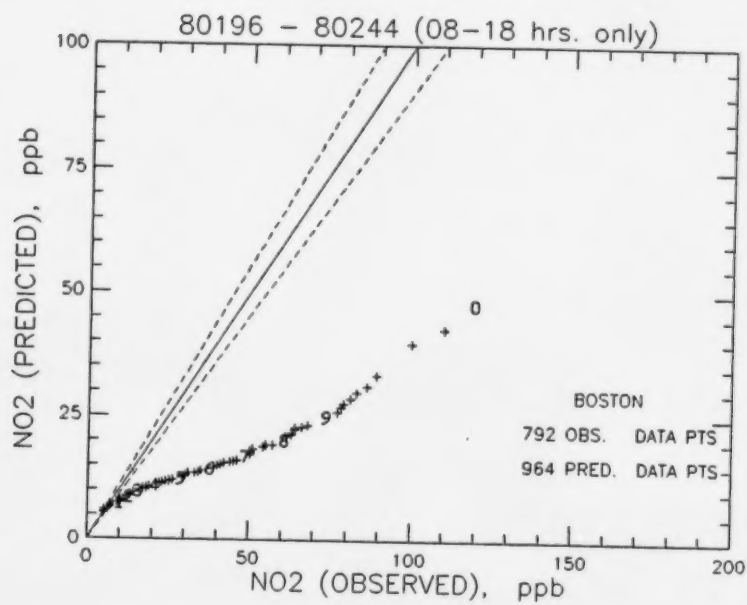
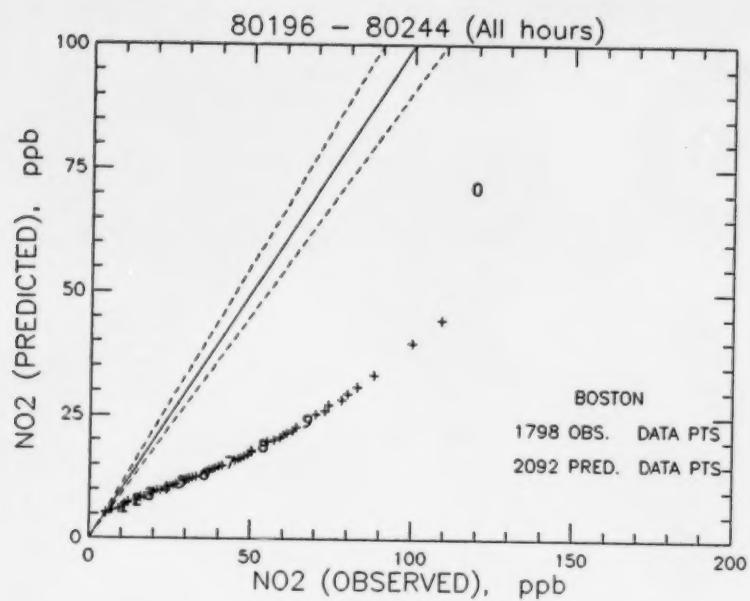


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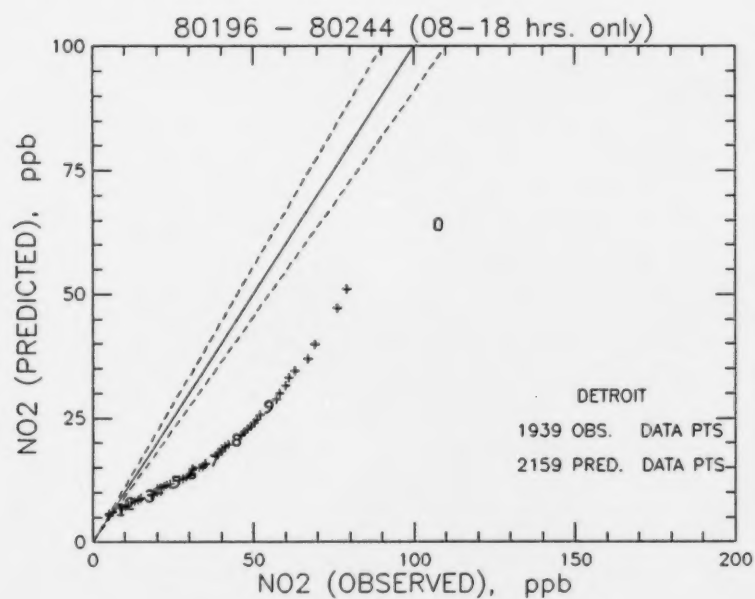
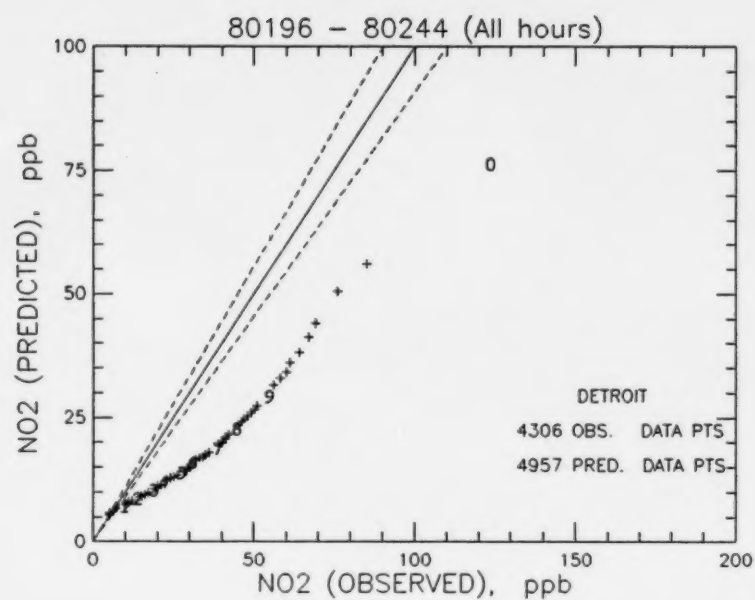


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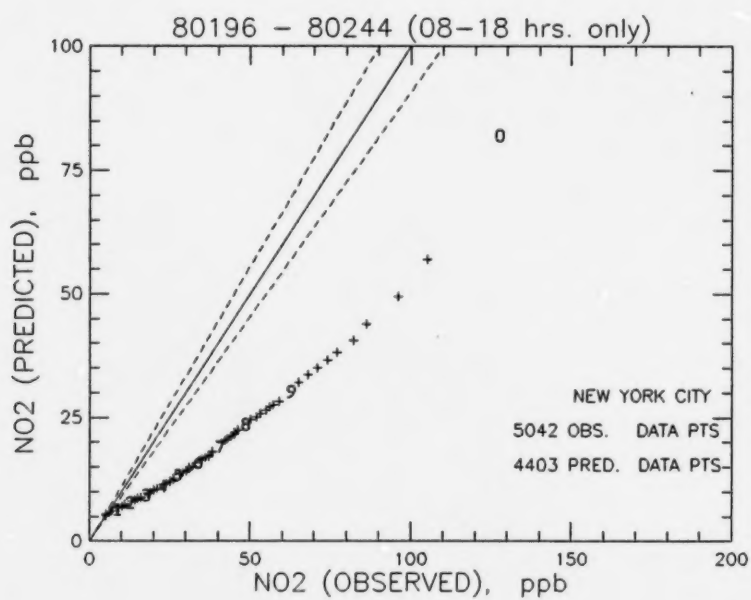
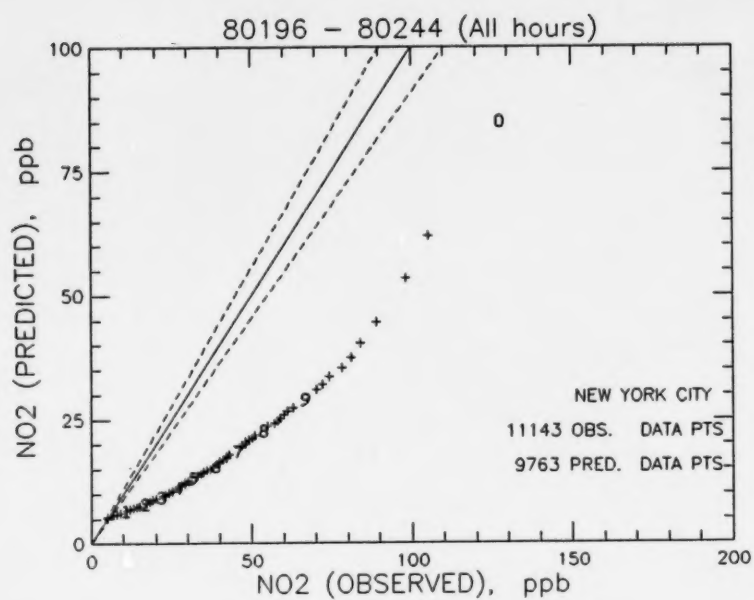


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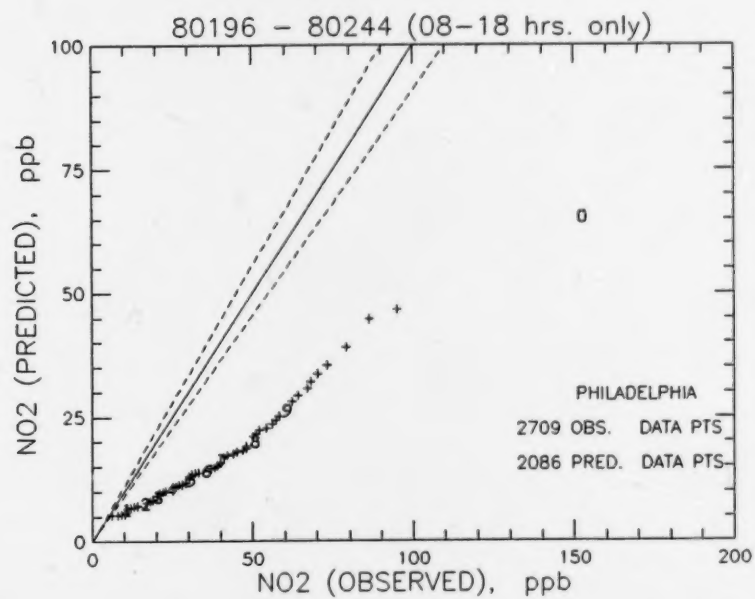
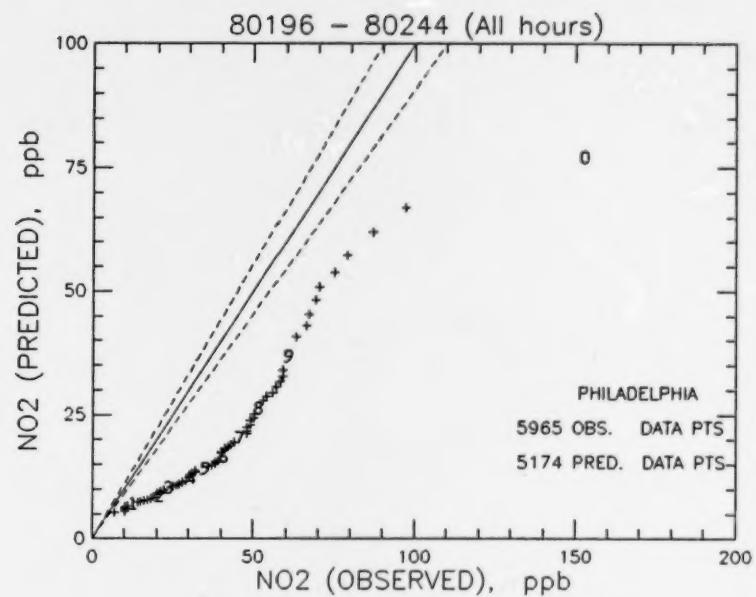


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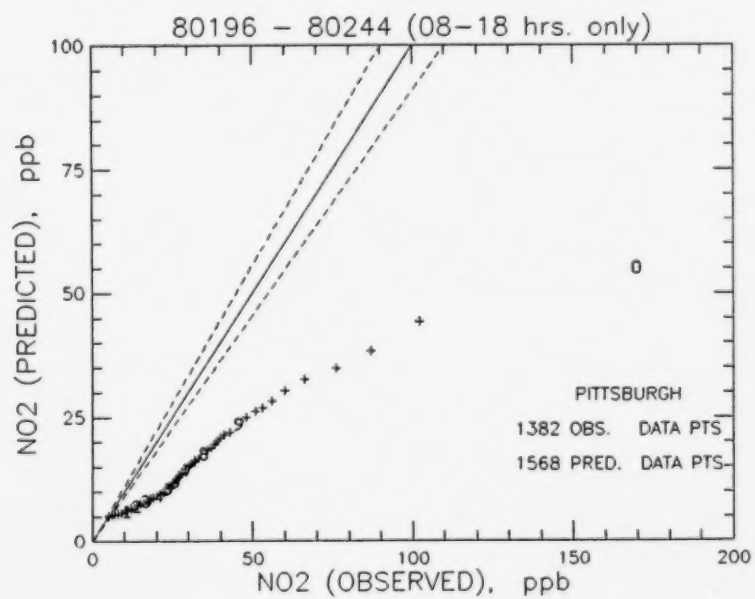
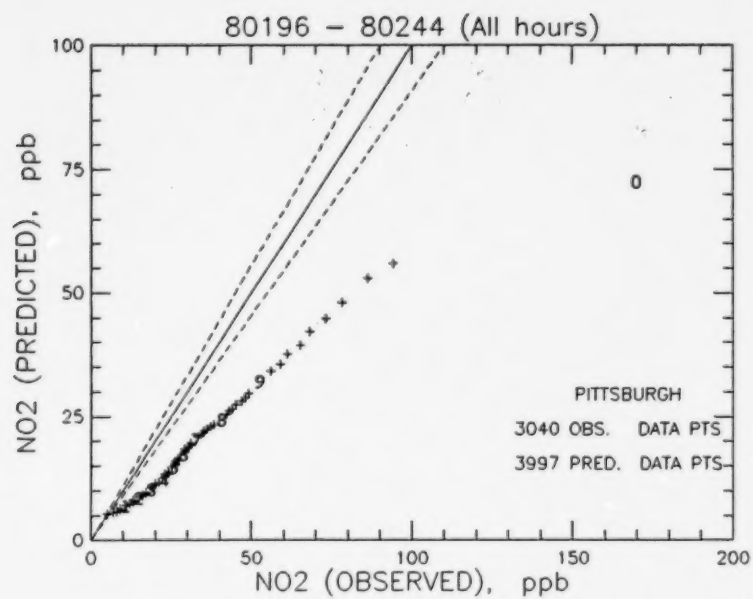


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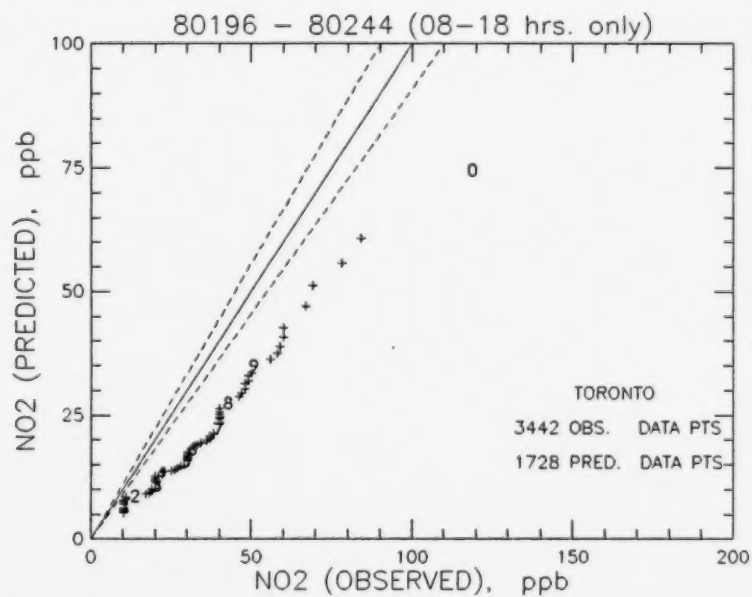
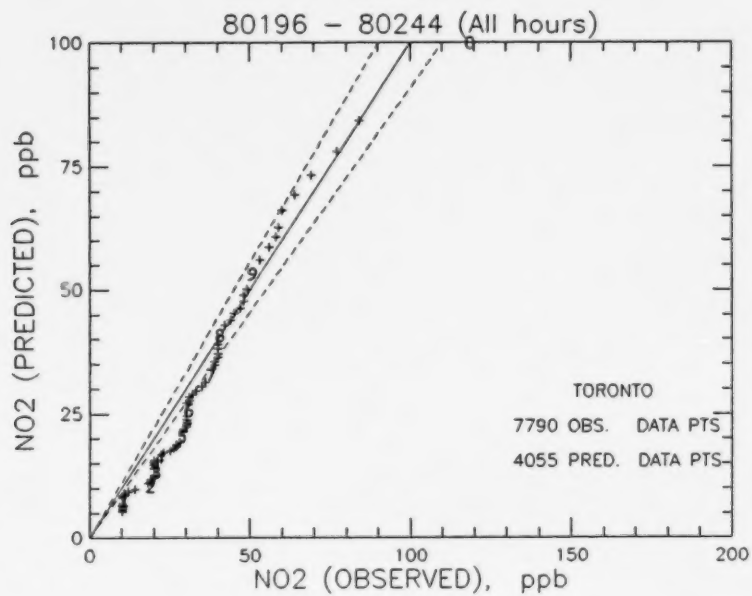


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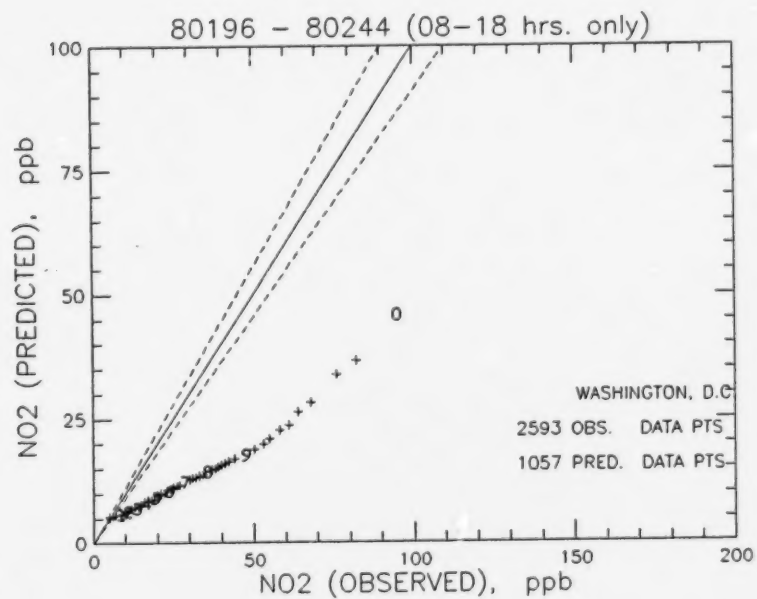
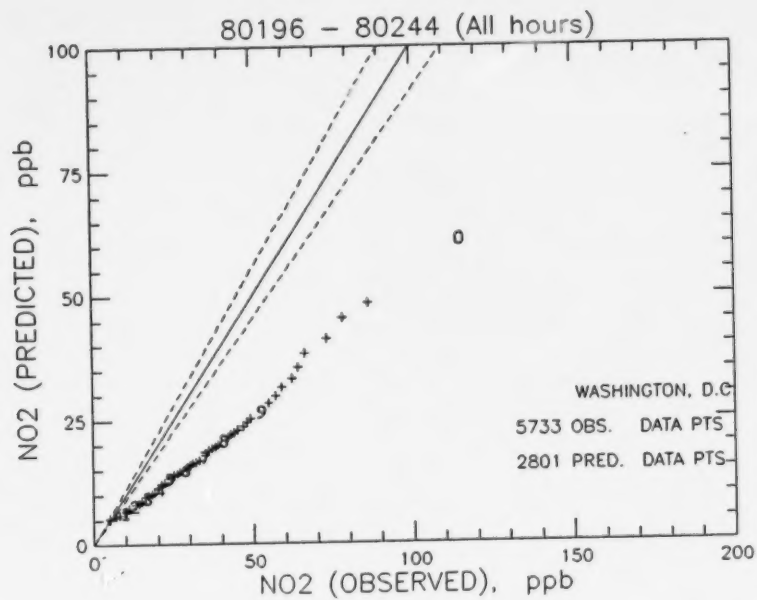
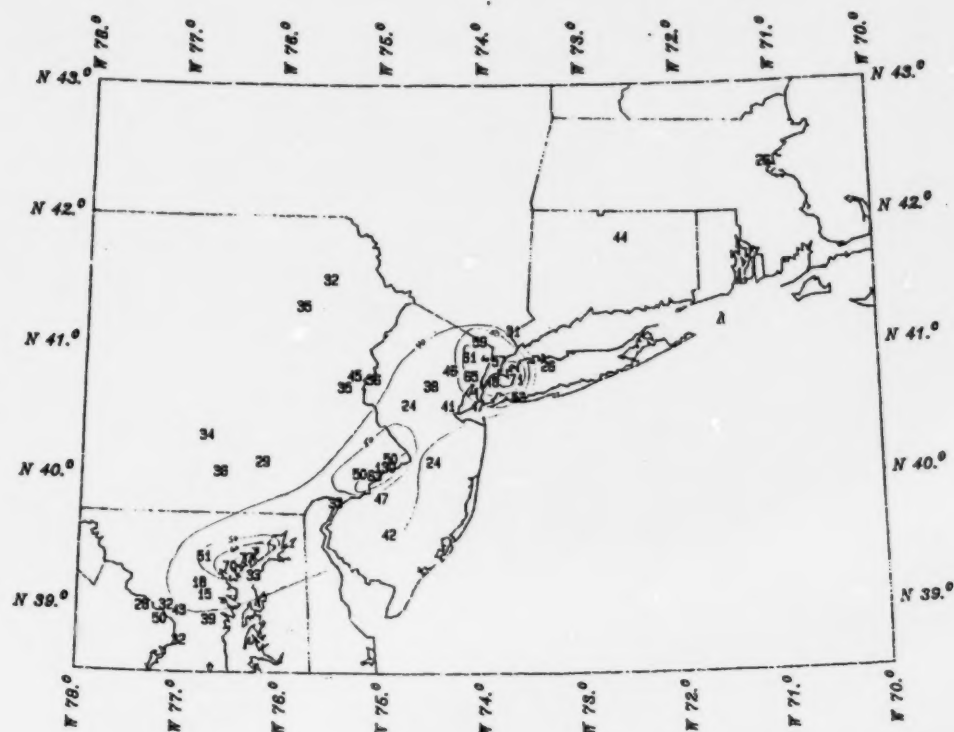


Figure 6.6. (continued)

(a)



(b)

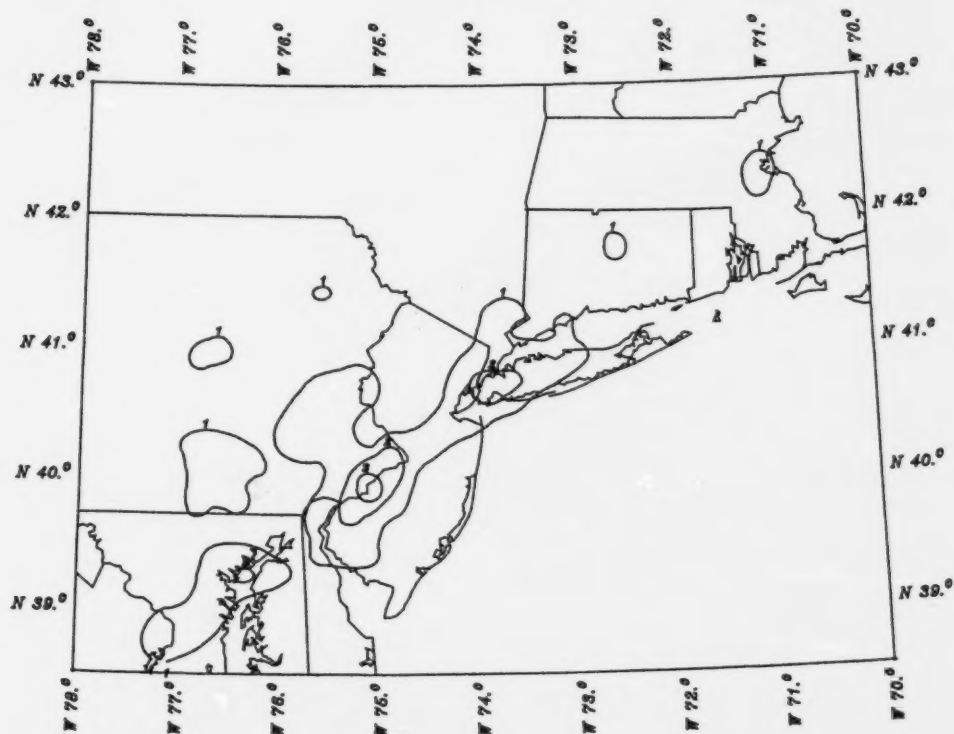


Figure 6.7. Fields of maximum 05–08 h, LST average concentrations over the period July 14–17, 1980 of (a) observed NO_2 , (b) predicted NO_2 , (c) observed NO_x , and (d) predicted NO_x . Observed data are in concentration units of ppb, predicted NO_2 data are in units of ppb/10 and predicted NO_x data are in units of ppb/100.

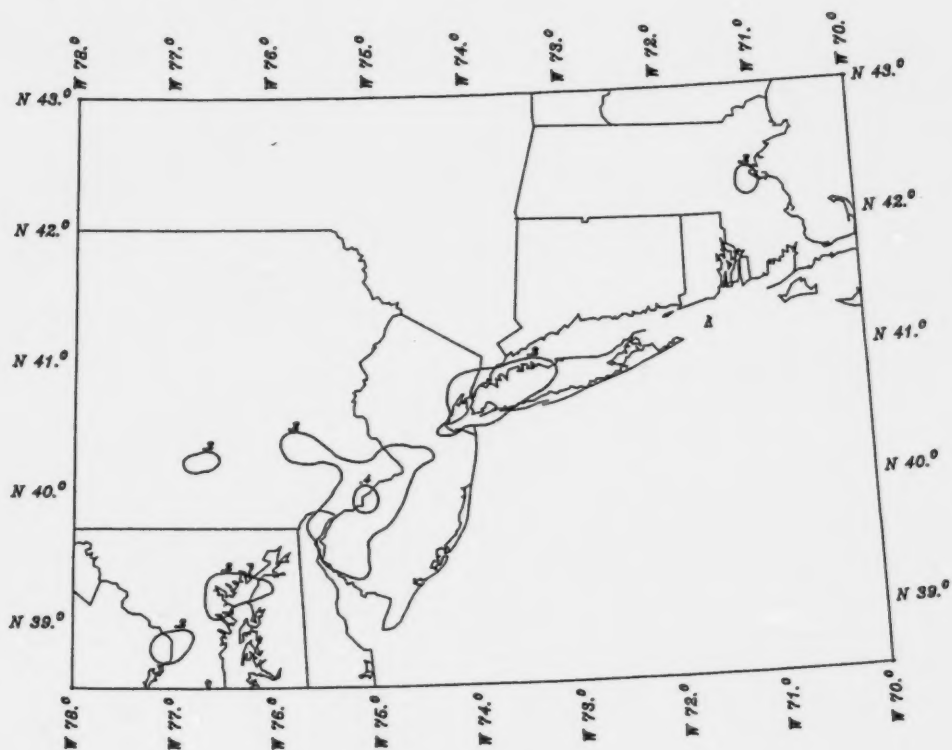
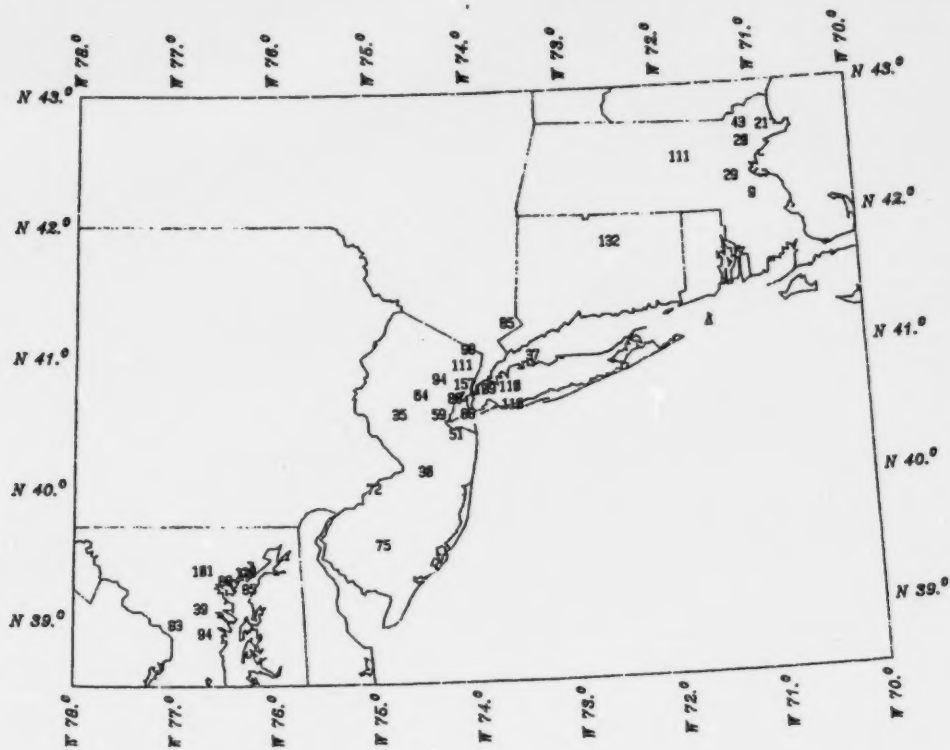
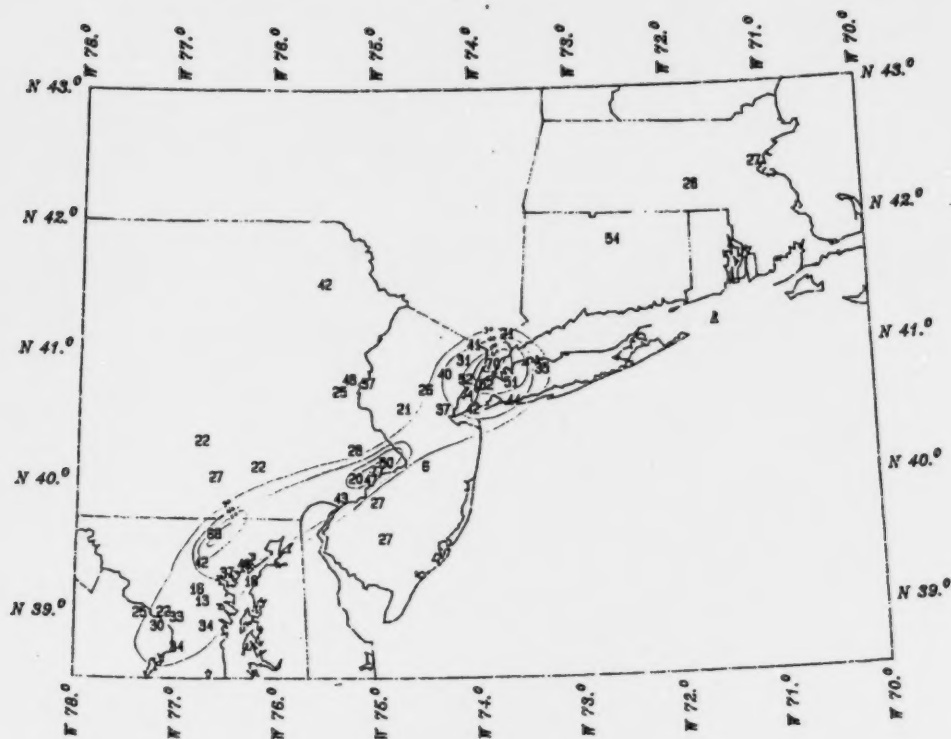


Figure 6.7. (continued)

(a)



(b)

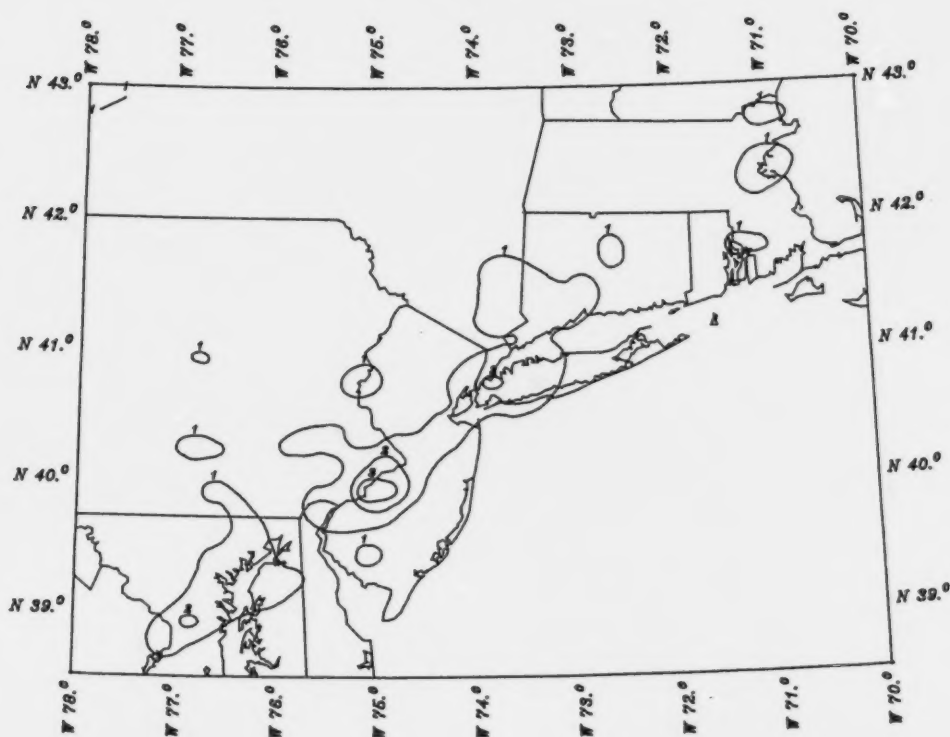
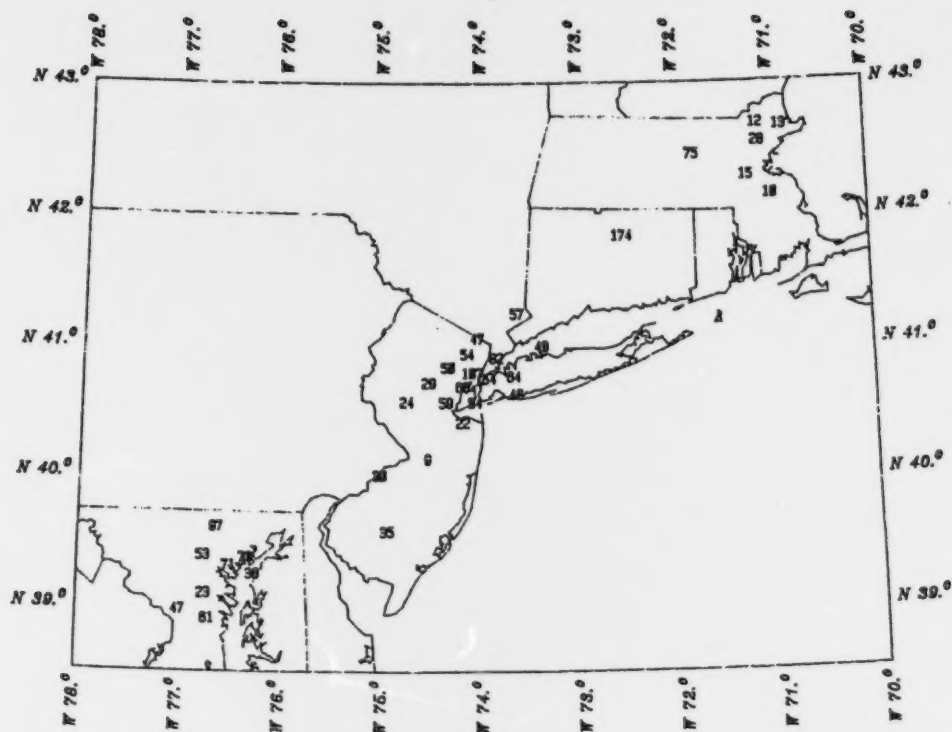


Figure 6.8. Fields of maximum 05–08 h, LST average concentrations over the period July 20–22, 1980 of (a) observed NO_2 , (b) predicted NO_2 , (c) observed NO_x , and (d) predicted NO_x . Observed data are in concentration units of ppb, predicted NO_2 data are in units of ppb/10 and predicted NO_x data are in units of ppb/100.

(c)



(d)

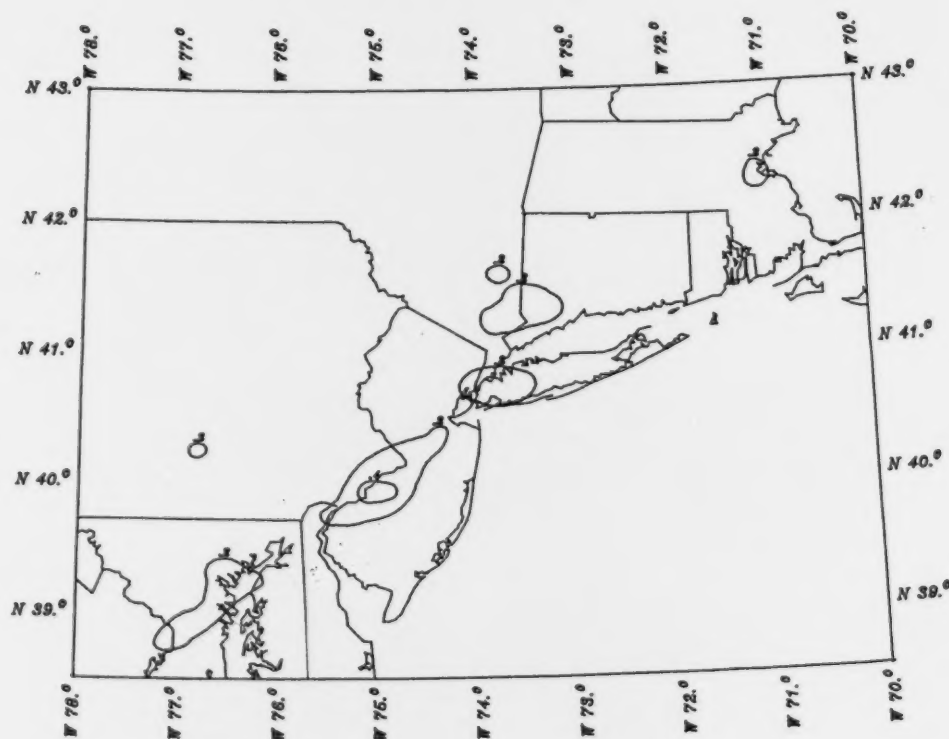


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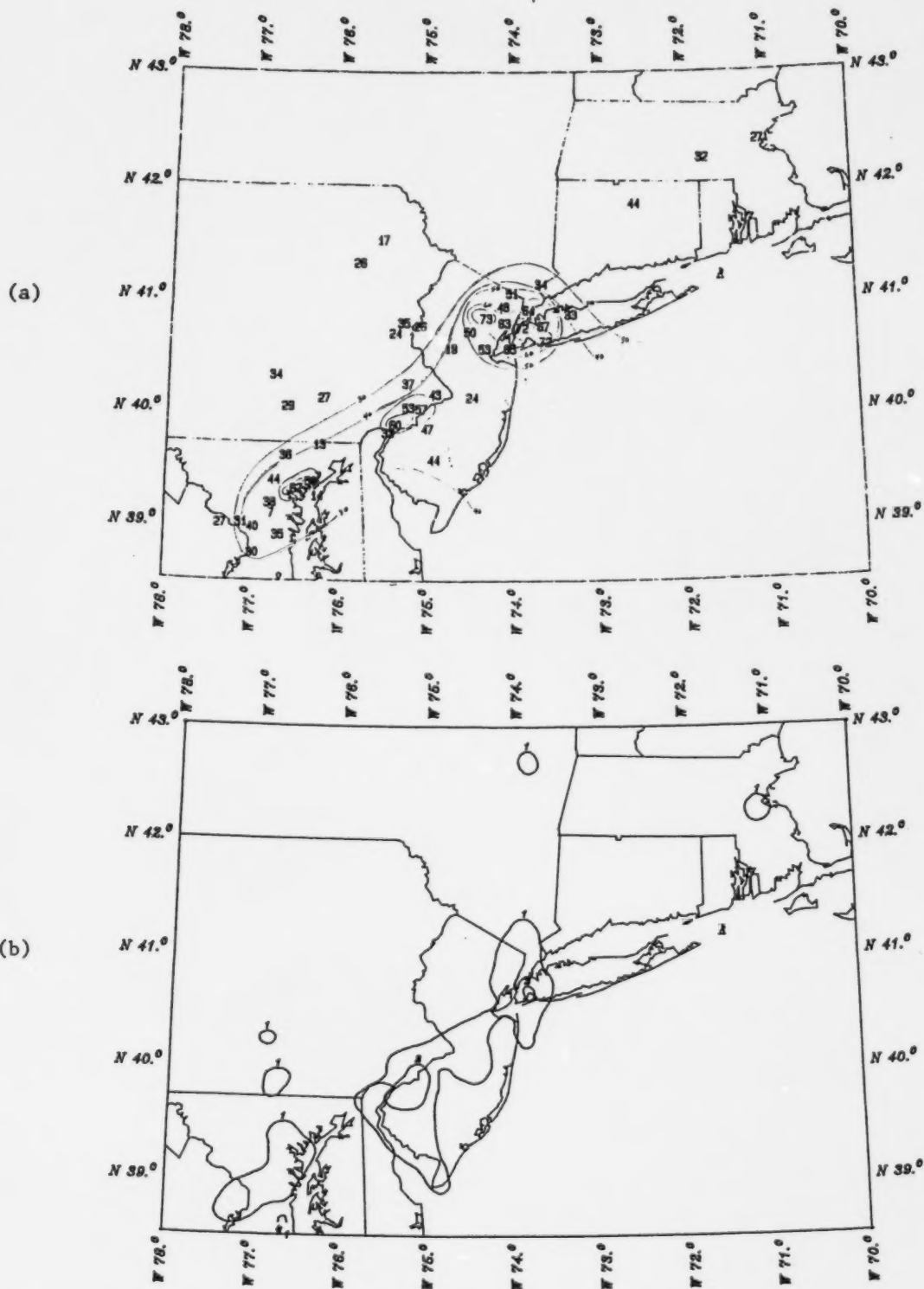


Figure 6.9. Fields of maximum 05-08 h, LST average concentrations over the period July 25-27, 1980 of (a) observed NO_2 , (b) predicted NO_2 , (c) observed NO_x , and (d) predicted NO_x . Observed data are in concentration units of ppb, predicted NO_2 data are in units of ppb/10 and predicted NO_x data are in units of ppb/100.

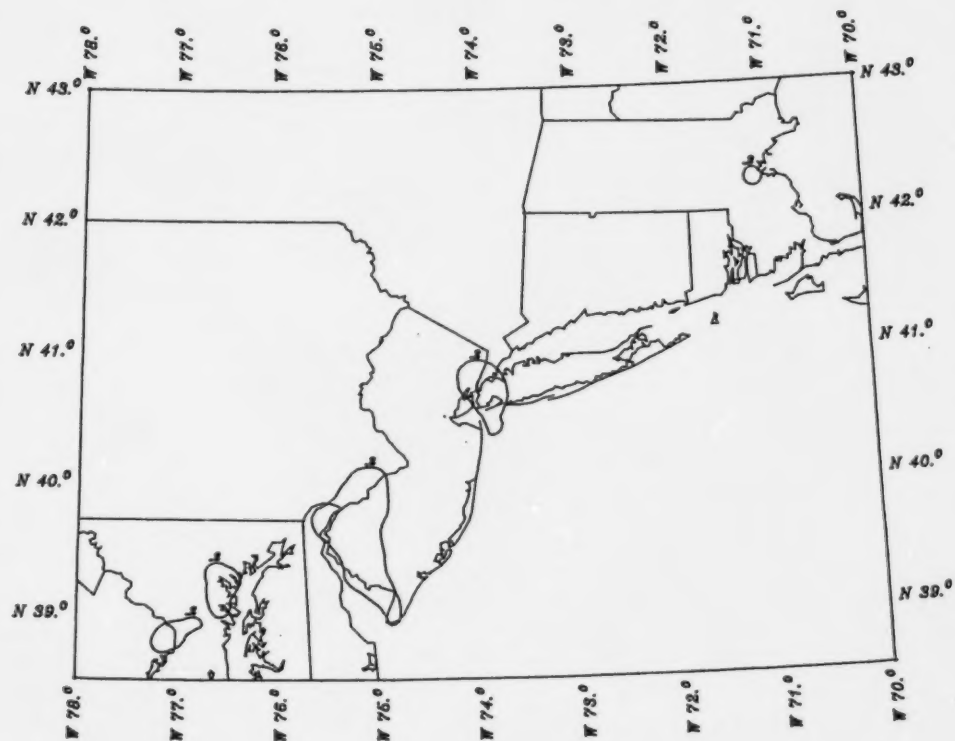
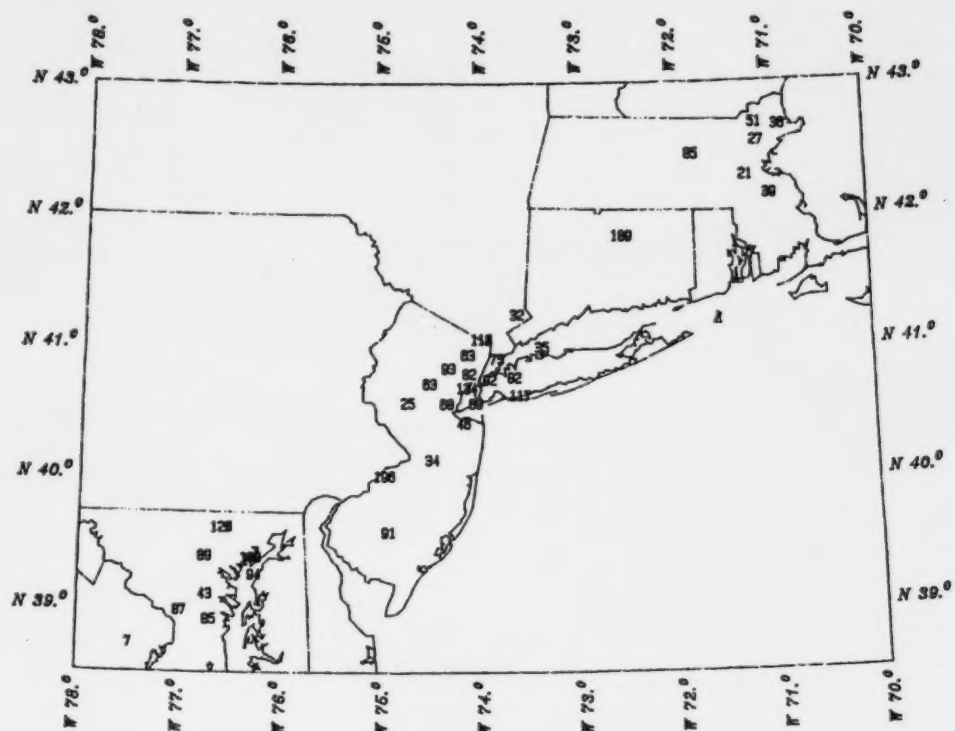


Figure 6.9. (continued)

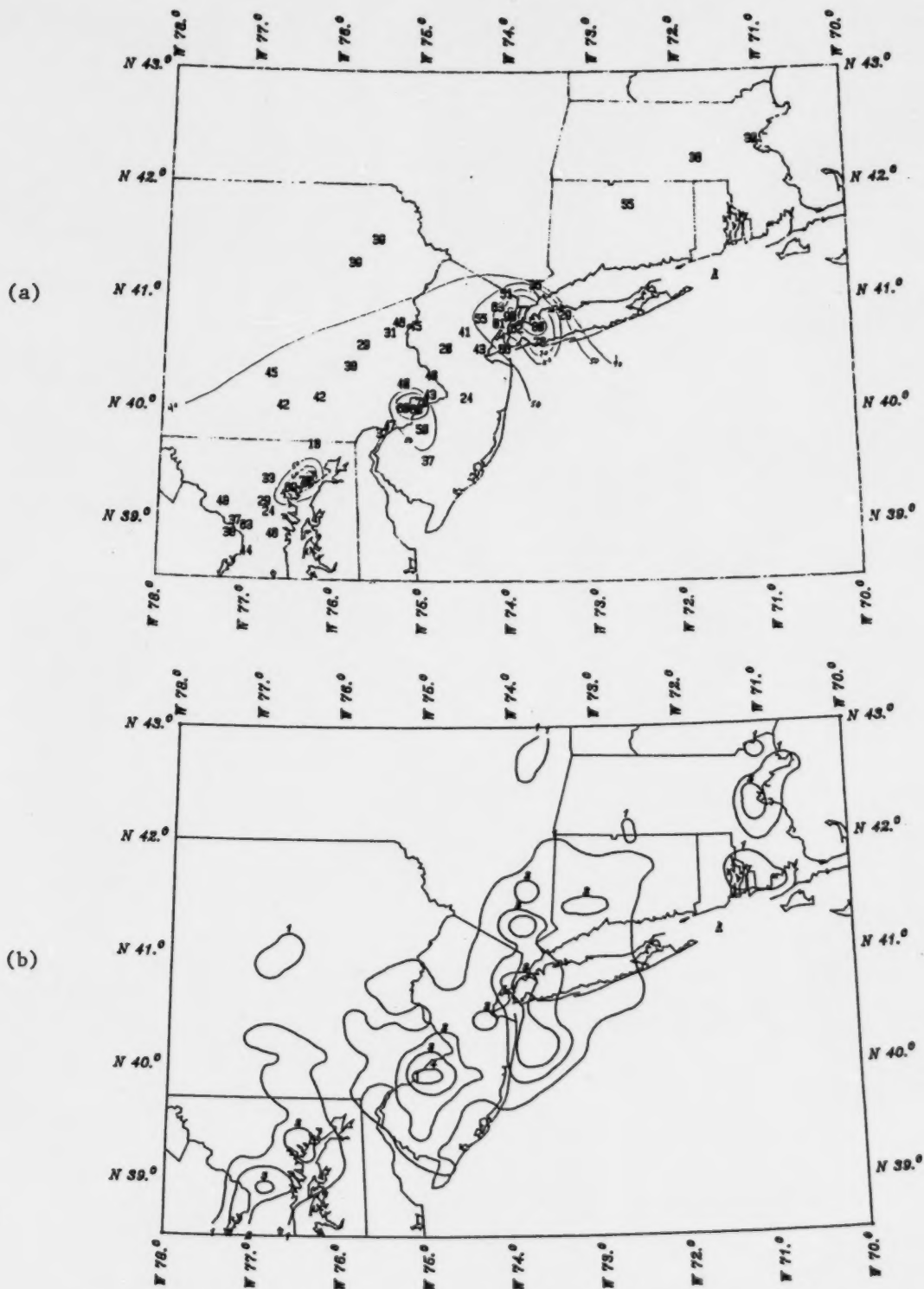
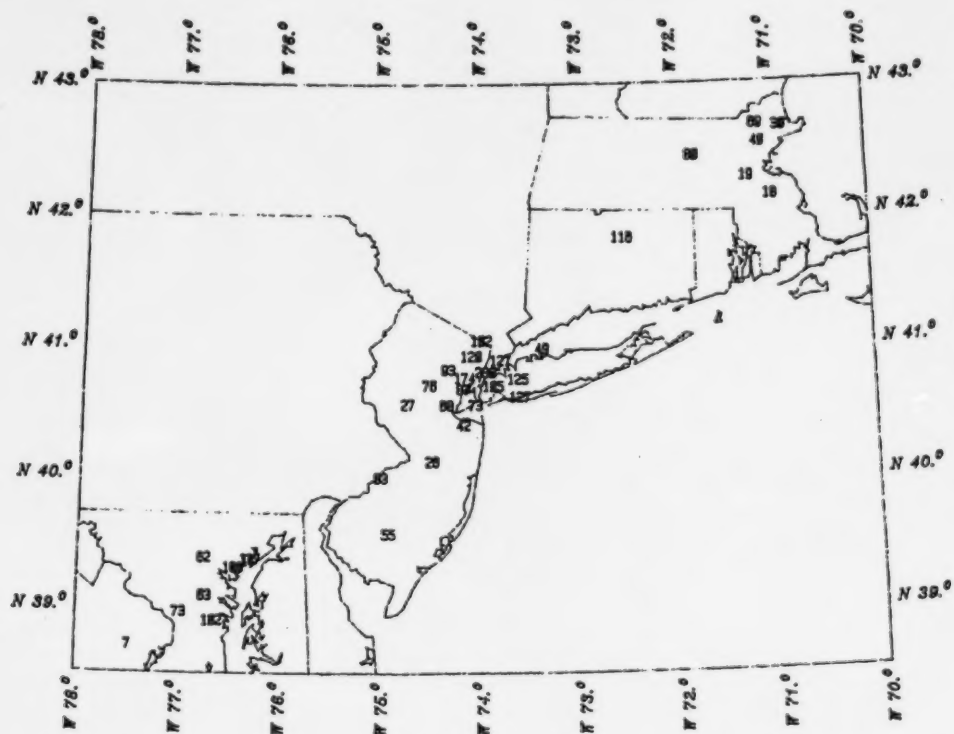


Figure 6.10. Fields of maximum 05-08 h, LST average concentrations over the period July 30-August 8, 1980 of (a) observed NO_2 , (b) predicted NO_2 , (c) observed NO_x , and (d) predicted NO_x . Observed data are in concentration units of ppb, predicted NO_2 data are in units of ppb/10 and predicted NO_x data are in units of ppb/100.

(c)



(d)

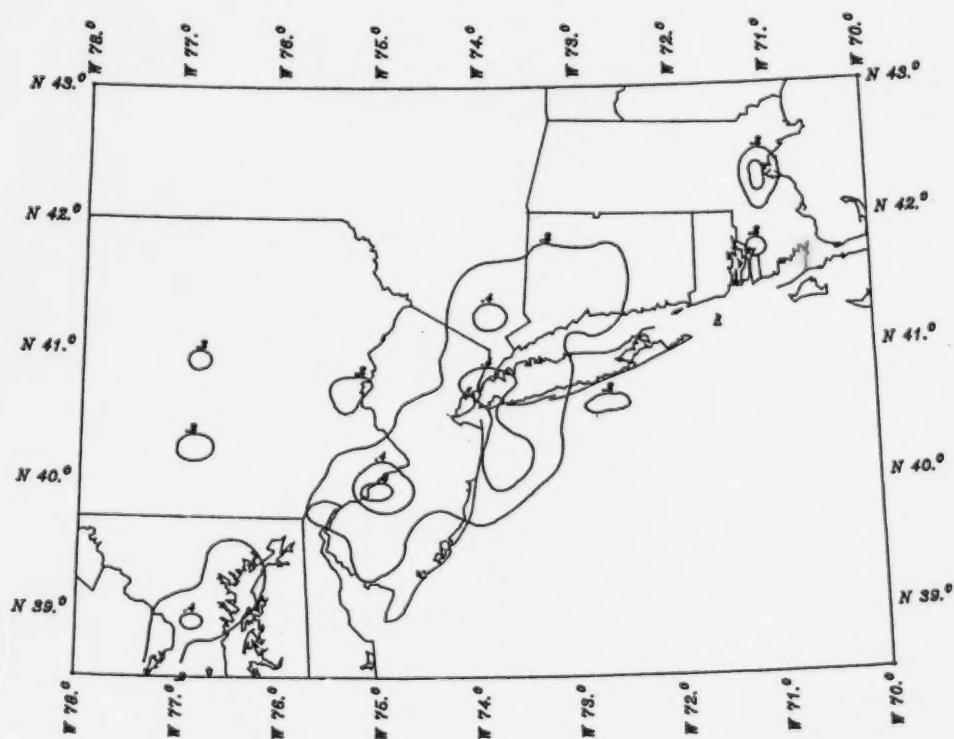
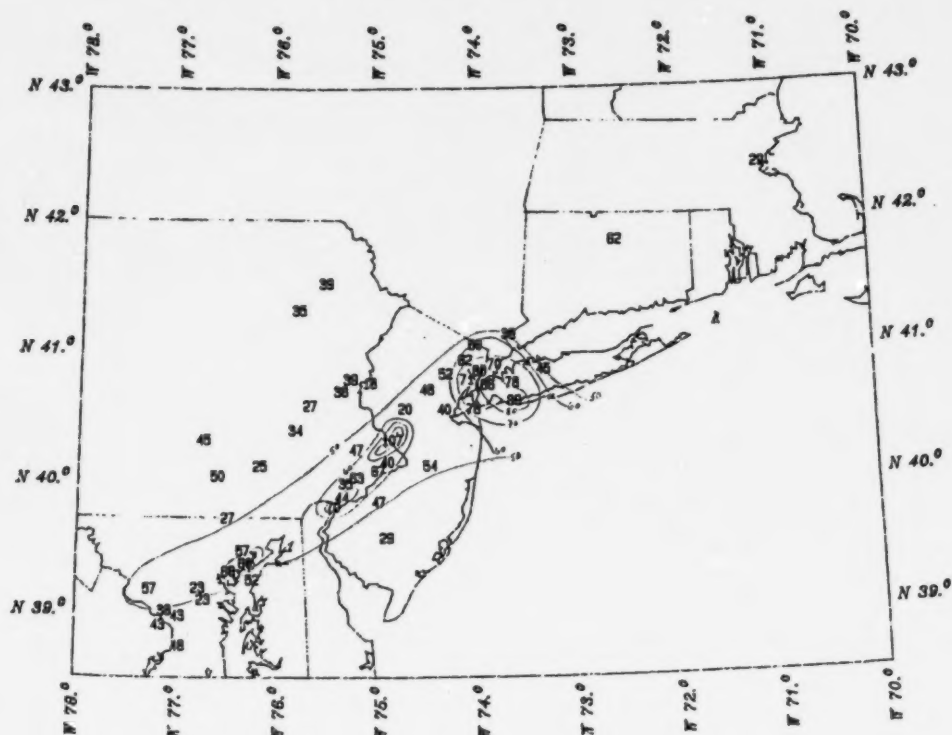


Figure 6.10. (continued)

(a)



(b)

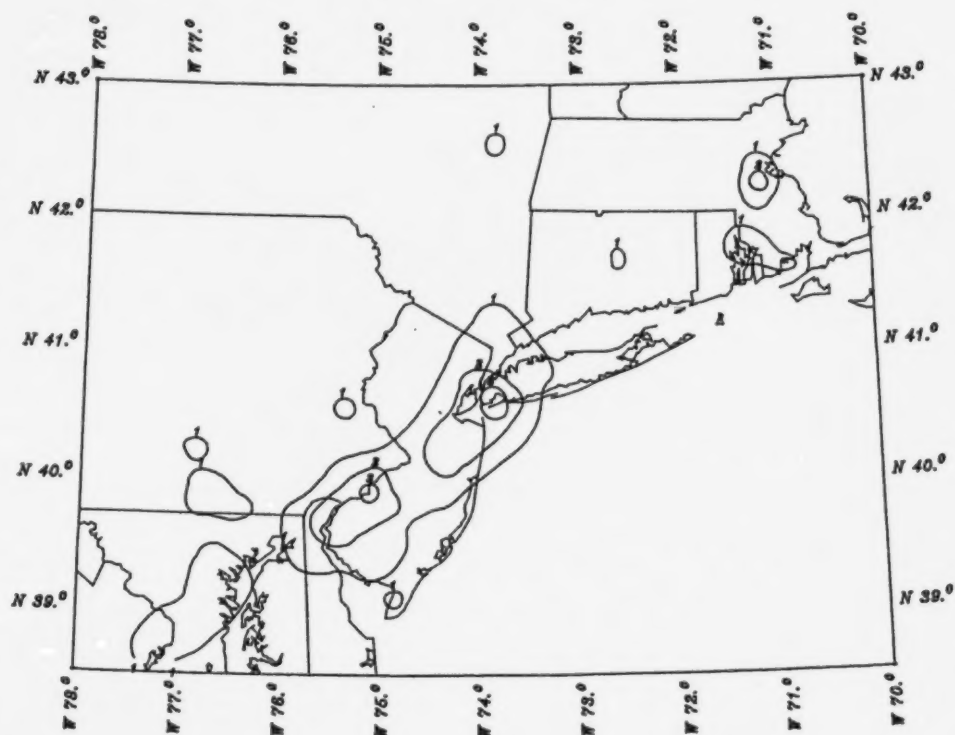
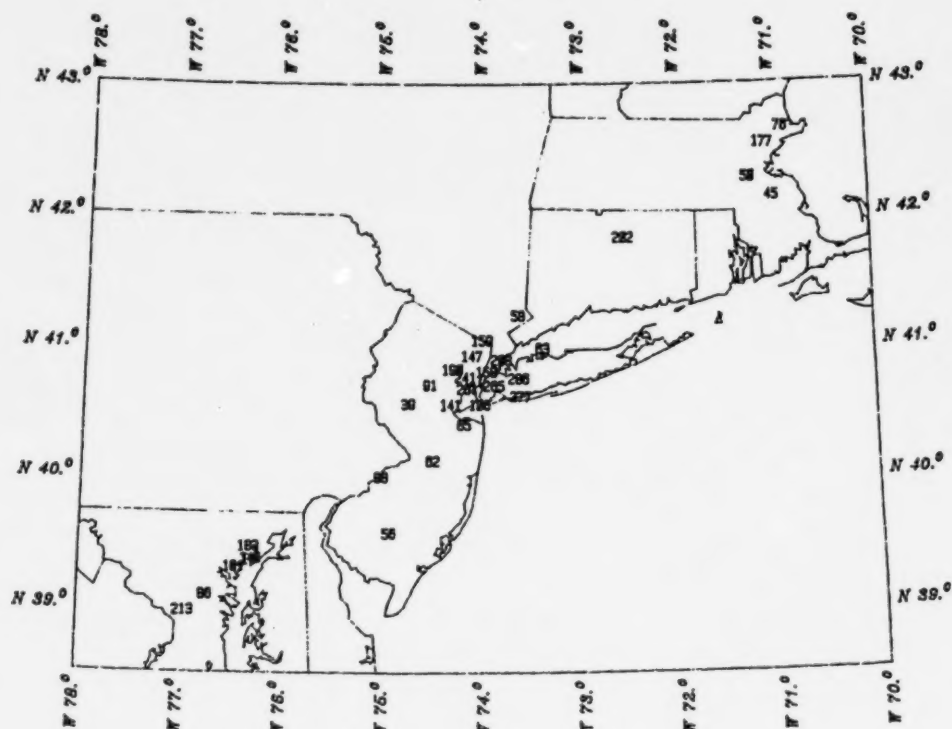


Figure 6.11. Fields of maximum 05-08 h, LST average concentrations over the period August 25-28, 1980 of (a) observed NO_2 , (b) predicted NO_2 , (c) observed NO_x , and (d) predicted NO_x . Observed data are in concentration units of ppb, predicted NO_2 data are in units of ppb/10 and predicted NO_x data are in units of ppb/100.

(c)



(d)

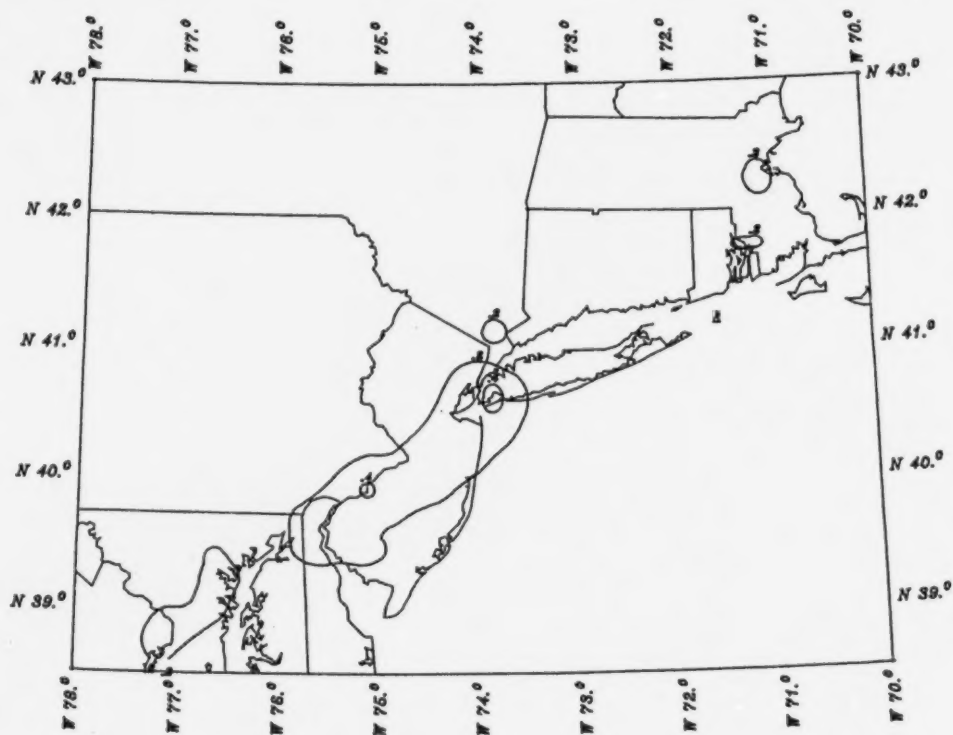


Figure 6.11. (continued)

7 EVALUATION OF SURFACE-BASED NMHC

7.1 DATA PREPARATION

7.1.1 Surface Sampling Sites

Routine surface monitoring for non-methane hydrocarbons (NMHC) in the Northeast U.S. is usually not performed because of the expense and difficulty in obtaining high quality data in short time. However, during the 1980 summer season the intensive NEROS and NECRMP field programs sponsored special data collection efforts of surface NMHCs in the Northeast (Richter, 1983 and Vaughan, 1985). These data were collected in stainless steel canisters and subsequently analyzed in laboratories by gas chromatograph. This analysis provides quantitative information on specific organic compounds found in the collected sample.

The NEROS hydrocarbon samples were obtained in the Columbus, OH and Baltimore-Washington areas, generally during the afternoon hours, although a few samples were taken in the morning as well. These samples were collected in downwind areas within one-day travel time of the nearby urban centers. The NECRMP samples were collected within major urban centers of the Northeast Corridor in the 6-9 a.m.(LDT) morning period. These samples are thought to be most representative of the local organic emissions distribution in the urban center. Table 7.1 lists the locations of the sampling sites, the number of samples obtained at each location during the field program, and the agency responsible for performing the sampling. Individual samples generally represent one-hour integrated collections within a canister.

Unlike the evaluation analyses for O_3 , NO_2 , and NO_x discussed in previous sections, the ROM evaluation for NMHC is more diagnostic than operational. There are a number of reasons for this. First, the intermittency of the data poses some problems in setting up evaluative tests. The NMHC data are sparse in both space and time. Group aggregations, as performed for the other species, are more difficult

to perform here. The samples are not very regionally representative because of the location of the sampling sites and the very reactive nature of some of the organic components in the samples. Also, the chromatographic analysis does not show quantitative data for the oxygenated organics, such as formaldehyde and acetaldehyde, which are components of the NMHC variable. Therefore, the comparisons of ROM predictions and observations of NMHC are presented in a deterministic manner for diagnostic purposes to show whether there is a clear systematic bias in the way in which the ROM predictions of NMHC compare with observations. Close statistical comparison of the data set is not warranted. Also, spatial pattern comparisons will not be made because the observed data set is insufficient to determine spatial gradients of NMHC on the regional scale.

TABLE 7.1. SUMMARY OF SURFACE-BASED SAMPLES OF NMHC
OBTAINED DURING THE 1980 SUMMER PERIOD

Sampling Site	# Samples Obtained	Agency
<u>Columbus, OH area</u>		
Ft. Hayes, OH	58	U.S. EPA
West Jefferson, OH	28	U.S. EPA
North Albany, OH	36	U.S. EPA
<u>Baltimore, MD area</u>		
Read St.	82	Washington State Univ.
Essex, MD	90	Washington State Univ.
<u>Washington, DC area</u>		
West End Library	60	Washington State Univ.
Takoma Park School	16	Washington State Univ.
College Park, MD	44	Washington State Univ.
<u>Downwind of Wash.-Balt. area</u>		
Mobile van - BNL	43	Brookhaven National Lab.
Mobile van - WSU	20	Washington State Univ.
<u>Northern New Jersey</u>		
Linden, NJ	81	Washington State Univ.
Newark, NJ	71	Washington State Univ.
<u>Boston, MA area</u>		
East Boston, MA	85	Battelle Columbus Labs.
Watertown, MA	90	Battelle Columbus Labs.

7.1.2 Data Reduction

The chromatographic analysis of each hydrocarbon canister results in a profile of concentrations of individual identifiable organic species as well as the concentrations of those organics that were detected but were not readily identifiable (unknowns). The unknown component in the 1980 analyzed samples typically varied from 10–20% on a carbon-mole basis. Samples in which there was interference or bad data at particular peaks on the chromatographic spectrum were not included in this analysis. Next, the carbon concentrations of the individual organics were summed according to their membership in several reactivity classes used in the Carbon Bond 4 (CB-4) chemical kinetic mechanism (Gery *et al.*, 1988). This is the mechanism used in the ROM to simulate atmospheric photochemistry. These reactivity classes are based on reacting carbon structures within an organic molecule, and include ethylene (ETH), olefins (OLE), paraffins (PAR), formaldehyde (FORM), higher aldehydes (ALD2), toluene-like aromatics (TOL), xylene-like aromatics (XYL), isoprene (ISOP), and non reactivities other than methane (NONR). Rather than ignoring the unknown component, we distributed the mass of the unknown organics proportionally into the CB-4 reactivity classes according to the carbon weightings of the known components. In apportioning the individual organics to the CB-4 classes the units were changed from a carbon basis to a compound basis for comparison with model results because the ROM reactivity class predictions are on a compound basis. Also, the concentrations were summed on a carbon basis to provide the total NMHC for comparison with the analogous ROM-predicted quantity. Table 7.2 presents an example of the steps in processing the chromatographic results of a single canister sample. The results of the analysis of samples taken within the same ROM grid cell and for the same day and hour were averaged. Results of samples taken within the 6–9 a.m. period were also averaged for a given grid cell.

The ROM predicts the concentrations (ppb) of hydrocarbon species for each of the above nine reactivity classes contained in the CB-4 chemical mechanism. Results for the appropriate grid cell and hour (or block of hours, as is the case for the 6–9 a.m. time period) were selected to compare with the measured data. To obtain values of the NMHC variable from the ROM predictions, a carbon-weighted sum of the concentrations from each of the individual reactivity classes was performed:

$$\begin{aligned} NMHC(ppbC) = & 2 * ETH + 2 * OLE + PAR + FORM + 2 * ALD2 \\ & + 7 * TOL + 8 * XYL + 4 * ISOP + NONR \end{aligned}$$

Predicted results for the same grid cell where the measurement was taken, as well as the average of the 9-cell block centered on the cell where the measurement was taken were calculated. The purpose of using the latter prediction is to compare the result of the local ROM performance with a slightly expanded area, allowing as much latitude as possible in comparing the observation with the prediction.

TABLE 7.2. EXAMPLE OF PROCESSING A HYDROCARBON CANISTER
SAMPLE (EAST BOSTON, MA SITE - 80197 - 0800 h)

DATA FROM CHROMATOGRAPHIC ANALYSIS			
Species Name	ppbC	Species Name	ppbC
Ethane	14.0	3-Methylhexane	7.5
Ethylene	38.5	2,2,4-Trimethylpentane	6.5
Acetylene	23.0	N-Heptane	6.5
Propane	12.5	Ethylcyclopentane	4.0
Propene	4.0	2,4-Dimethylhexane	2.0
I-Butane	17.0	Toluene	47.5
N-butane	59.5	2-Methylheptane	3.0
T-2-Butene	3.0	3-Methylheptane	4.0
C-2-Butene	2.0	N-Octane	3.0
I-Pentane	60.5	Ethylbenzene	9.0
N-Pentane	33.5	P-Xylene	28.5
2,3-Dimethylbutane	7.5	O-Xylene	11.0
2-Methylpentane	19.0	N-Propylbenzene	1.0
3-Methylpentane +	12.5	M-Ethyltoluene +	5.0
Cyclohexane		P-Ethyltoluene	
N-Hexane	13.0	1,3,5-Trimethylbenzene	3.5
Methylcyclopentane	6.5	O-Ethyltoluene	1.5
Cyclopentane +	3.5	1,2,4-Trimethylbenzene	11.5
2,4-Dimethylpentane		1,2,3-Trimethylbenzene	1.5
Benzene	15.0	Unknowns	67.0
2-Methylhexane	7.0		
Total Knowns = 508 ppbC (88%)		Total Unknowns = 67 ppbC (12%)	

KNOWN SPECIES CONCENTRATIONS DISTRIBUTED INTO
CB-4 REACTIVITY CLASSES

CB-4 Class	ppb	%-Carbon of Total Knowns	CB-4 Class	ppb	%-Carbon of Total Knowns
ETH	19.25	7.52	TOL	8.02	10.97
OLE	1.33	0.52	XYL	7.49	11.71
PAR	308.27	60.21	ISOP	-	-
FORM	-	-	NONR	41.45	8.10
ALD2	2.50	0.98			

TABLE 7.2. (continued)
FINAL SPECIES CONCENTRATIONS DISTRIBUTED INTO
CB-4 REACTIVITY CLASSES (Unknowns distributed
to maintain same %-carbon as in knowns)

CB-4 Class	ppb	CB-4 Class	ppb
ETH	21.77	TOL	9.07
OLE	1.50	XYL	8.47
PAR	348.61	ISOP	-
FORM	-	NONR	46.88
ALD2	2.83		

There is an inherent bias built into the comparison from the start. The chromatographic technique used to analyze the observed hydrocarbon samples does not detect the oxygenated organics, such as formaldehyde and acetaldehyde. The non-zero concentrations of the oxygenated reactivity classes of the CB-4 mechanism for the observed samples derives from atomic structures in non-oxygenated organic compounds, detected by the chromatograph, that "act" like the oxygenates as far as reactivity is concerned. However, the majority of true oxygenates are missing from the observed value, and this can amount to $\approx 5\%$ or more of the mass of organics on a carbon basis. Hence, in the comparisons of NMHC that follow, the observed concentrations should be increased by this amount, on average, to compensate for the missing oxygenated component. In practice, for the analysis to follow, *this missing component was not added into total observed NMHC.*

7.2 RESULTS

Results of the hydrocarbon analysis for samples collected in the 06-09 a.m. period are presented in Table 7.3. The data are divided by geographic area and further subdivided by location within ROM grid cells. The date and grid cell location are indicated in the first three columns of the table. Data from all samples taken within the grid cell and within the specified time period for the date are averaged. The number of such samples is indicated in the fourth column. The average observed NMHC concentration (O) is listed in the fifth column. The predicted concentration from the same grid cell and time period (P1) is shown in the sixth column, and the predicted 9-cell average (P2) is given in the seventh column. The ratios of $O/P1$ and $O/P2$ are presented in the remaining columns.

The differences in the P1 and P2 predictions are attributable to spatial concentration gradients in the vicinity of the grid cell containing the sampling site. Where P1 is from a center city location, P1 is typically larger than P2. When P1 is outside the center city, P2 is usually larger since it includes the major urban

TABLE 7.3. SUMMARY OF AVERAGED 06-09 h (LDT) NMHC CONCENTRATIONS, OBSERVED AND PREDICTED

DATE	COL	ROW	N	NMHC(O) (ppbC)	NMHC(P1) (ppbC)	NMHC(P2) (ppbC)	O/P1 RATIO	O/P2 RATIO
Columbus, OH area:								
80202	3	12	1	117.10	48.41	62.34	2.42	1.88
80203	3	12	1	90.34	61.69	72.63	1.46	1.24
80207	3	12	3	173.92	44.41	54.58	3.92	3.19
80208	3	12	4	163.85	42.04	47.29	3.90	3.46
80213	3	12	2	99.72	31.51	33.34	3.16	2.99
80218	3	12	2	28.51	44.22	47.81	0.64	0.60
AVERAGES:				112.24	45.38	53.00	2.58	2.23
Columbus, OH area:								
80202	5	12	2	315.76	93.51	86.86	3.38	3.64
80208	5	12	1	380.38	91.77	60.78	4.14	6.26
80213	5	12	1	689.78	88.21	53.83	7.82	12.81
80217	5	12	2	1026.12	107.83	63.91	9.52	16.06
80221	5	12	2	625.82	124.16	77.56	5.04	8.07
80226	5	12	2	1123.37	144.03	65.48	7.80	17.16
AVERAGES:				693.54	108.25	68.07	6.28	10.66
Columbus, OH area:								
80207	5	13	4	117.76	144.56	94.07	0.81	1.25
80213	5	13	1	329.37	106.49	59.01	3.09	5.58
AVERAGES:				223.57	125.52	76.54	1.95	3.42
Washington, DC area:								
80196	28	6	1	186.86	151.32	105.62	1.23	1.77
80198	28	6	1	883.13	149.42	126.74	5.91	6.97
80200	28	6	1	763.66	122.81	83.93	6.22	9.10
80203	28	6	1	306.67	133.36	119.44	2.30	2.57
80204	28	6	1	739.15	134.00	146.60	5.52	5.04
80205	28	6	1	322.56	97.99	133.97	3.29	2.41
80207	28	6	2	884.87	149.44	94.91	5.92	9.32
80212	28	6	1	520.74	113.69	78.40	4.58	6.64
80213	28	6	2	821.16	144.64	86.87	5.68	9.45
80214	28	6	1	571.24	161.60	128.26	3.53	4.45
80219	28	6	2	1400.54	225.34	153.25	6.22	9.14
80220	28	6	2	785.27	146.52	161.54	5.36	4.86
80221	28	6	2	864.21	160.04	136.11	5.40	6.35
80225	28	6	1	970.45	169.35	149.51	5.73	6.49
80228	28	6	1	1598.44	129.79	143.07	12.32	11.17
80232	28	6	1	2824.15	152.50	128.70	18.52	21.94
80233	28	6	1	191.02	136.12	111.13	1.40	1.72
80234	28	6	2	794.11	221.33	166.20	3.59	4.78
80235	28	6	1	3652.56	305.77	225.71	11.95	16.18
80239	28	6	1	1106.27	229.91	142.41	4.81	7.77
80240	28	6	1	1398.86	145.76	96.34	9.60	14.52
80242	28	6	2	1245.99	151.78	111.63	8.21	11.16
AVERAGES:				1037.81	160.57	128.65	6.24	7.90

TABLE 7.3. (continued)

DATE	COL	ROW	N	NMHC(O) (ppbC)	NMHC(P1) (ppbC)	NMHC(P2) (ppbC)	O/P1 RATIO	O/P2 RATIO
Washington, DC area:								
80210	29	7	2	319.25	111.10	97.86	2.87	3.26
80211	29	7	1	875.66	181.54	213.00	4.82	4.11
80212	29	7	2	456.70	72.37	95.50	6.31	4.78
80213	29	7	2	774.46	75.90	106.95	10.20	7.24
80214	29	7	2	743.89	119.18	147.13	6.24	5.06
80217	29	7	1	353.00	83.98	96.56	4.20	3.66
80219	29	7	2	421.07	167.56	196.31	2.51	2.14
80220	29	7	1	886.61	257.43	193.50	3.44	4.58
80221	29	7	2	1042.05	116.49	150.67	8.95	6.92
80224	29	7	2	536.24	228.09	256.21	2.35	2.09
80225	29	7	2	895.74	195.85	191.90	4.57	4.67
80226	29	7	1	485.40	67.24	92.29	7.22	5.26
80227	29	7	2	1085.68	101.14	121.67	10.73	8.92
80228	29	7	2	1075.45	144.72	175.26	7.43	6.14
80231	29	7	2	241.25	178.53	162.71	1.35	1.48
80232	29	7	2	761.64	129.56	156.09	5.88	4.88
80233	29	7	1	623.57	134.57	149.15	4.63	4.18
80234	29	7	2	288.45	126.17	153.39	2.29	1.88
80235	29	7	2	259.89	254.29	287.59	1.02	0.90
80238	29	7	2	512.54	111.43	120.75	4.60	4.24
80239	29	7	2	896.76	144.69	158.70	6.20	5.65
80240	29	7	2	1418.01	93.64	113.47	15.14	12.50
80241	29	7	2	1670.77	88.64	120.40	18.85	13.88
80242	29	7	1	1157.52	122.12	133.08	9.48	8.70
AVERAGES:				740.90	137.76	153.76	6.30	5.30
Washington, DC area:								
80200	30	7	1	262.40	132.01	101.65	1.99	2.58 *
AVERAGES:				262.40	132.01	101.65	1.99	2.58

TABLE 7.3. (continued)

DATE	COL	ROW	N	NMHC(O) (ppbC)	NMHC(P1) (ppbC)	NMHC(P2) (ppbC)	O/P1 RATIO	O/P2 RATIO
Baltimore, MD area:								
80196	30	8	1	242.99	156.48	83.98	1.55	2.89
80201	30	8	2	1053.13	216.38	123.62	4.87	8.52
80202	30	8	1	379.59	204.14	165.39	1.86	2.30
80203	30	8	1	489.95	173.48	150.49	2.82	3.26
80205	30	8	2	652.49	125.94	151.95	5.18	4.29
80206	30	8	1	179.34	154.93	99.87	1.16	1.80
80208	30	8	1	605.24	144.80	95.89	4.18	6.31
80209	30	8	1	378.64	140.08	114.24	2.70	3.31
80210	30	8	2	885.74	131.51	86.51	6.73	10.24
80211	30	8	1	516.23	250.49	200.35	2.06	2.58
80212	30	8	2	415.80	144.92	88.22	2.87	4.71
80213	30	8	1	853.48	165.29	95.31	5.16	8.95
80218	30	8	1	430.56	215.79	185.22	2.00	2.32
80220	30	8	2	750.55	172.55	155.74	4.35	4.82
80221	30	8	1	672.74	175.13	144.12	3.84	4.67
80222	30	8	2	383.05	193.41	135.92	1.98	2.82
80224	30	8	2	797.23	512.02	219.32	1.56	3.64
80225	30	8	2	676.32	223.52	196.46	3.03	3.44
80226	30	8	1	461.04	137.23	85.50	3.36	5.39
80226	30	8	2	575.51	137.23	85.50	4.19	6.73
80227	30	8	2	1476.74	161.73	111.55	9.13	13.24
80228	30	8	2	846.62	154.95	187.01	5.46	4.53
80229	30	8	2	189.35	113.58	104.64	1.67	1.81
80231	30	8	2	659.49	155.99	162.85	4.23	4.05
80232	30	8	2	1429.59	196.73	152.20	7.27	9.39
80233	30	8	2	767.76	220.68	127.04	3.48	6.04
80234	30	8	2	465.22	186.48	138.83	2.49	3.35
80235	30	8	3	1243.55	395.93	305.33	3.14	4.07
80236	30	8	2	776.28	220.58	147.37	3.52	5.27
80237	30	8	2	319.58	138.21	83.91	2.31	3.81
80238	30	8	1	562.05	163.79	103.68	3.43	5.42
80239	30	8	2	845.59	211.76	129.09	3.99	6.55
80240	30	8	2	1347.83	159.59	100.59	8.45	13.40
80241	30	8	2	638.17	169.68	111.15	3.76	5.74
80242	30	8	2	734.63	176.28	114.62	4.17	6.41
AVERAGES:				677.20	188.61	135.53	3.77	5.32

TABLE 7.3. (continued)

DATE	COL	ROW	N	NMHC(O) (ppbC)	NMHC(P1) (ppbC)	NMHC(P2) (ppbC)	O/P1 RATIO	O/P2 RATIO
Baltimore, MD area:								
80196	31	8	1	1068.42	47.21	72.43	22.63	14.75
80197	31	8	2	375.26	142.41	144.29	2.64	2.60
80198	31	8	2	756.63	103.57	144.72	7.31	5.23
80199	31	8	2	400.58	196.07	190.96	2.04	2.10
80200	31	8	2	457.08	81.86	91.83	5.58	4.98
80201	31	8	2	1230.67	79.30	105.59	15.52	11.66
80202	31	8	2	453.83	147.54	155.56	3.08	2.92
80203	31	8	2	629.99	111.63	155.28	5.64	4.06
80204	31	8	2	821.22	127.94	151.42	6.42	5.42
80205	31	8	2	724.39	109.64	163.88	6.61	4.42
80206	31	8	1	403.91	80.48	94.27	5.02	4.28
80207	31	8	1	218.15	85.52	93.10	2.55	2.34 *
80208	31	8	1	350.68	77.72	89.13	4.51	3.93
80212	31	8	1	421.87	80.65	86.28	5.23	4.89
80218	31	8	1	613.12	153.54	167.50	3.99	3.66
80220	31	8	1	436.43	113.54	135.32	3.84	3.23
80224	31	8	1	1320.25	129.85	189.06	10.17	6.98
80235	31	8	2	226.31	368.44	345.18	0.61	0.66
80236	31	8	2	552.44	113.89	168.87	4.85	3.27
80237	31	8	2	290.19	63.82	82.20	4.55	3.53
80238	31	8	2	793.02	76.97	103.18	10.30	7.69
80239	31	8	2	964.59	99.91	117.97	9.65	8.18
80240	31	8	2	2195.89	82.36	93.75	26.66	23.42
80241	31	8	2	1604.29	113.82	109.48	14.09	14.65
80242	31	8	2	605.55	99.10	115.13	6.11	5.26
AVERAGES:				716.59	115.47	134.66	7.58	6.16
Baltimore, MD area:								
80201	31	9	1	714.34	88.61	103.14	8.06	6.93
80203	31	9	1	357.65	162.33	149.51	2.20	2.39 *
AVERAGES:				535.99	125.47	126.32	5.13	4.66

TABLE 7.3. (continued)

DATE	COL	ROW	N	NMHC(O) (ppbC)	NMHC(P1) (ppbC)	NMHC(P2) (ppbC)	O/P1 RATIO	O/P2 RATIO
New York, NY area:								
80196	39	16	2	516.69	103.40	88.47	5.00	5.84
80199	39	16	1	798.65	123.82	138.39	6.45	5.77
80201	39	16	2	802.98	89.27	89.20	9.00	9.00
80204	39	16	1	330.79	116.47	124.44	2.84	2.66
80206	39	16	2	906.31	109.41	103.71	8.28	8.74
80207	39	16	2	868.74	80.73	80.93	10.76	10.73
80208	39	16	1	543.46	54.30	63.34	10.01	8.58
80210	39	16	2	712.96	114.95	92.19	6.20	7.73
80211	39	16	2	957.97	109.89	105.64	8.72	9.07
80212	39	16	2	1072.63	118.46	111.89	9.05	9.59
80213	39	16	2	969.20	111.33	93.84	8.71	10.33
80214	39	16	2	2988.65	113.76	135.86	26.27	22.00
80215	39	16	2	604.08	93.77	112.42	6.44	5.37
80217	39	16	2	1319.73	94.37	100.18	13.98	13.17
80218	39	16	1	1165.87	185.35	201.32	6.29	5.79
80224	39	16	2	2155.43	142.55	187.24	15.12	11.51
80225	39	16	2	675.48	172.99	193.86	3.90	3.48
80235	39	16	1	811.03	192.25	174.56	4.22	4.65
80238	39	16	2	679.42	133.93	117.96	5.07	5.76
80239	39	16	1	3503.64	100.53	116.98	34.85	29.95
80240	39	16	1	1782.60	93.46	99.42	19.07	17.93
80242	39	16	1	100.46	91.04	131.67	1.10	0.76
AVERAGES:				1103.04	115.73	121.07	10.06	9.47

TABLE 7.3. (continued)

DATE	COL	ROW	N	NMHC(O) (ppbC)	NMHC(P1) (ppbC)	NMHC(P2) (ppbC)	O/P1 RATIO	O/P2 RATIO
New York, NY area:								
80198	40	17	2	512.82	137.00	146.25	3.74	3.51
80199	40	17	2	540.21	159.85	145.55	3.38	3.71
80200	40	17	1	452.81	150.64	133.52	3.01	3.39
80201	40	17	2	1220.26	110.50	99.51	11.04	12.26
80202	40	17	2	403.91	75.17	95.43	5.37	4.23
80203	40	17	2	617.39	134.56	130.88	4.59	4.72
80204	40	17	2	333.25	129.50	132.26	2.57	2.52
80205	40	17	2	478.40	136.31	149.16	3.51	3.21
80206	40	17	2	312.95	145.28	122.82	2.15	2.55
80207	40	17	2	440.58	115.44	102.05	3.82	4.32
80208	40	17	2	332.51	77.00	71.01	4.32	4.68
80210	40	17	2	401.82	165.17	120.08	2.43	3.35
80211	40	17	2	760.47	139.32	129.08	5.46	5.89
80212	40	17	2	481.11	170.46	147.31	2.82	3.27
80213	40	17	2	680.54	140.59	127.74	4.84	5.33
80214	40	17	2	752.52	187.34	163.45	4.02	4.60
80215	40	17	2	303.74	96.62	100.25	3.14	3.03
80217	40	17	2	859.82	140.54	126.70	6.12	6.79
80218	40	17	2	1880.60	261.40	214.49	7.19	8.77
80219	40	17	1	567.58	222.53	215.35	2.55	2.64
80220	40	17	2	475.40	152.74	147.44	3.11	3.22
80221	40	17	2	797.63	128.56	142.50	6.20	5.60
80222	40	17	2	217.45	83.58	99.18	2.60	2.19
80224	40	17	2	255.68	150.39	165.35	1.70	1.55
80225	40	17	2	510.32	177.11	184.66	2.88	2.76
80226	40	17	1	245.27	121.61	120.12	2.02	2.04
80231	40	17	2	345.32	189.22	161.37	1.82	2.14
80232	40	17	2	441.84	277.79	254.40	1.59	1.74
80233	40	17	2	729.12	380.92	295.07	1.91	2.47
80234	40	17	2	434.24	263.15	247.34	1.65	1.76
80235	40	17	2	294.12	204.69	187.25	1.44	1.57
80236	40	17	2	344.94	111.17	104.50	3.10	3.30
80238	40	17	2	228.33	163.46	136.22	1.40	1.68
80239	40	17	2	1540.25	147.93	136.96	10.41	11.25
80240	40	17	2	708.35	133.25	126.68	5.32	5.59
80241	40	17	2	478.18	141.80	144.89	3.37	3.30
80242	40	17	2	480.13	146.72	160.56	3.27	2.99
AVERAGES:				563.78	158.63	148.31	3.78	4.00

TABLE 7.3. (continued)

DATE	COL	ROW	N	NMHC(O) (ppbC)	NMHC(P1) (ppbC)	NMHC(P2) (ppbC)	O/P1 RATIO	O/P2 RATIO
Boston, MA area:								
80196	52	27	4	331.10	109.88	83.99	3.01	3.94
80197	52	27	4	322.74	113.11	91.49	2.85	3.53
80198	52	27	3	373.51	168.94	139.06	2.21	2.69
80199	52	27	4	485.46	136.61	117.72	3.55	4.12
80200	52	27	4	372.55	114.49	86.19	3.25	4.32
80201	52	27	4	188.49	70.50	59.72	2.67	3.16
80202	52	27	2	195.85	84.09	70.34	2.33	2.78
80203	52	27	2	549.37	155.76	174.40	3.53	3.15
80205	52	27	3	239.03	199.98	186.07	1.20	1.28
80206	52	27	2	252.29	126.66	88.76	1.99	2.84
80207	52	27	3	375.63	102.61	75.99	3.66	4.94
80208	52	27	4	393.40	62.77	57.45	6.27	6.85
80209	52	27	4	477.00	83.53	62.28	5.71	7.66
80211	52	27	4	295.94	146.70	96.43	2.02	3.07
80212	52	27	4	326.84	216.26	165.85	1.51	1.97
80213	52	27	4	284.25	93.01	67.56	3.06	4.21
80214	52	27	4	602.42	125.38	92.74	4.80	6.50
80215	52	27	4	346.17	131.67	146.27	2.63	2.37
80216	52	27	3	231.61	113.60	123.12	2.04	1.88
80217	52	27	4	660.77	126.29	95.67	5.23	6.91
80218	52	27	4	845.00	238.30	134.35	3.55	6.29
80219	52	27	4	394.82	219.40	169.13	1.80	2.33
80220	52	27	4	275.86	136.82	114.01	2.02	2.42
80221	52	27	4	589.39	152.54	116.31	3.86	5.07
80222	52	27	3	261.54	100.74	100.15	2.60	2.61
80223	52	27	5	186.81	85.21	73.76	2.19	2.53
80224	52	27	5	273.15	152.36	141.10	1.79	1.94
80225	52	27	5	393.27	367.65	300.77	1.07	1.31
80226	52	27	5	331.68	111.47	82.13	2.98	4.04
80227	52	27	4	1054.78	112.16	87.16	9.40	12.10
80228	52	27	4	970.08	157.72	166.02	6.15	5.84
80229	52	27	5	144.49	72.91	71.68	1.98	2.02
80230	52	27	5	153.21	59.14	59.76	2.59	2.56
80231	52	27	4	668.05	124.50	92.79	5.37	7.20
80232	52	27	5	197.69	179.30	139.60	1.10	1.42
80233	52	27	4	1541.44	186.70	121.11	8.26	12.73
80234	52	27	2	96.97	70.17	41.66	1.38	2.33
80235	52	27	3	1117.37	61.82	42.41	18.07	26.35
80236	52	27	4	628.75	71.61	61.49	8.78	10.23
80237	52	27	4	311.51	59.42	57.42	5.24	5.43
80238	52	27	4	1031.05	124.82	93.37	8.26	11.04
80239	52	27	4	2188.04	132.30	110.64	16.54	19.78
80240	52	27	4	648.39	110.13	100.39	5.89	6.46
80241	52	27	4	623.08	95.05	92.08	6.56	6.77
AVERAGES:				505.25	128.73	105.69	4.34	5.43

* Indicates that these data contain observations between the hours of 0600 and 0959 (LDT).

contribution. In any case the differences between P1 and P2 are much smaller than the differences between observed and predicted concentrations. Ratios of observed to predicted in the range of 4-7 are common in the larger urban areas. There is considerable scatter in the data from day to day for a given grid cell. The observed data span a wider range of values than the predicted data. This is illustrated in Figure 7.1 which presents scatter plots of the O and P1 data for each urban area. Unlike the comparisons for O_3 and NO_x , there does not appear to be a systematic trend toward increasing underprediction with increasing concentration. While nearly all the data are underpredicted, no clear trends are apparent.

NMHC data obtained outside of the 06-09 a.m. period are compared to predictions in Table 7.4 and Figure 7.2. The sampling locations for these data were in the Columbus, OH area and downwind of the Baltimore-Washington area. Concentrations at these late morning and afternoon times were generally lower than those from the early morning period. Many of these data were taken outside of the central urban area and may be more regionally representative than the urban-oriented 06-09 a.m. measurements. While the ROM predictions were still generally lower than the observations, the O/P ratios were improved in the later time period. Ratios of 1-3 were common.

The same sub-grid scale problems that tended to cause the ROM to underpredict NO_x and NO_2 concentrations will also cause underprediction for NMHC concentrations. The measurements are generally obtained in urban areas that are not representative of an entire ROM grid cell. Also, there are some components of the NMHC that are very reactive that may have been observed locally but that are essentially depleted by chemical reaction on the time and space scales of the model. There is probably yet another factor causing the degree of underprediction of the NMHCs to be worse than for the NO_x . While there is a high degree of uncertainty in the source emissions inventory for all species, it is particularly severe for the hydrocarbons (Langstaff and Wagner, 1986). Also, it is generally recognized that the emissions inventory for hydrocarbons is systematically biased low because of uninventoried sources and incorrect emissions factors. This underestimation of emissions has certainly added to the underprediction of NMHC.

Next, we examine several selected representative NMHC samples from the data base for comparisons among reactivity classes between the observed and predicted data. Appendix H lists the observed and predicted data selected for this analysis. Hydrocarbon data from several different days for each major urban area were included, as well as some data from the late morning-early afternoon period. NMHC concentrations (in ppbC) as well as the concentrations from individual reactivity classes (in ppb) and their associated carbon-mole percents are included in the data base. As indicated earlier, the oxygenated component of the observed data is essentially unmeasured by the chromatographic analysis. Therefore, to compensate for this discrepancy in the reactivity analysis, *we have added sufficient oxygenated*

TABLE 7.4. SUMMARY OF POST 06-09 h (LDT) NMHC CONCENTRATIONS,
OBSERVED AND PREDICTED HOURLY DATA

DATE	COL	ROW	HR	NMHC(O) (ppbC)	NMHC(P1) (ppbC)	NMHC(P2) (ppbC)	O/P1 RATIO	O/P2 RATIO
Columbus, OH area:								
80208	3	12	12	46.69	7.41	10.35	6.30	4.51
AVERAGES:				46.69	7.41	10.35	6.30	4.51
Columbus, OH area:								
80208	5	12	12	215.45	24.33	20.35	8.85	10.59
80203	5	12	13	114.39	28.96	18.53	3.95	6.17
80202	5	12	17	120.05	19.05	15.45	6.30	7.77
80203	5	12	20	149.49	69.13	51.14	2.16	2.92
AVERAGES:				149.85	35.37	26.37	5.32	6.86
Columbus, OH area:								
80208	5	13	12	240.68	30.75	22.26	7.83	10.81
AVERAGES:				240.68	30.75	22.26	7.83	10.81
Washington, DC area:								
80214	29	6	10	690.83	111.53	85.10	6.19	8.12
80203	29	6	11	217.96	116.03	75.41	1.88	2.89
80220	29	6	11	146.39	154.30	99.04	0.95	1.48
80221	29	6	11	104.99	104.88	100.74	1.00	1.04
80203	29	6	12	393.51	70.27	50.35	5.60	7.82
80213	29	6	12	158.88	85.60	60.69	1.86	2.62
80215	29	6	14	186.35	91.90	67.85	2.03	2.75
80207	29	6	15	325.67	81.34	61.40	4.00	5.30
AVERAGES:				278.07	101.98	75.07	2.94	4.00
Washington, DC area:								
80226	29	7	10	130.24	30.39	74.96	4.29	1.74
80214	29	7	11	204.92	39.44	70.31	5.20	2.91
80213	29	7	12	148.05	46.10	91.16	3.21	1.62
80221	29	7	12	101.08	75.85	88.27	1.33	1.15
80220	29	7	12	100.38	52.94	76.04	1.90	1.32
80215	29	7	15	477.21	65.38	76.62	7.30	6.23
80207	29	7	16	126.56	53.41	60.54	2.37	2.09
AVERAGES:				184.06	51.93	76.84	3.66	2.44
Washington, DC area:								
80200	30	7	10	216.18	133.82	79.57	1.62	2.72
80200	30	7	13	75.90	64.87	64.02	1.17	1.19
80206	30	7	14	47.31	49.12	35.28	0.96	1.34
80206	30	7	15	84.01	58.94	40.16	1.43	2.09
AVERAGES:				105.85	76.69	54.76	1.29	1.83

TABLE 7.4. (continued)

DATE	COL	ROW	HR	NMHC(O) (ppbC)	NMHC(P1) (ppbC)	NMHC(P2) (ppbC)	O/P1 RATIO	O/P2 RATIO
Baltimore, MD area:								
80209	30	9	10	119.84	95.78	58.44	1.25	2.05
80209	30	9	12	185.77	67.12	46.74	2.77	3.97
80209	30	9	15	334.90	48.54	33.81	6.90	9.91
80209	30	9	16	327.54	51.98	30.74	6.30	10.66
AVERAGES:				242.01	65.86	42.43	4.31	6.65
Baltimore, MD area:								
80220	31	7	10	172.26	39.80	76.76	4.33	2.24
80226	31	7	10	96.26	70.83	63.31	1.36	1.52
80220	31	7	12	57.57	32.09	47.63	1.79	1.21
80226	31	7	12	29.00	44.84	56.67	0.65	0.51
80220	31	7	14	70.49	45.67	63.44	1.54	1.11
80226	31	7	15	27.69	36.19	44.09	0.77	0.63
AVERAGES:				75.54	44.90	58.65	1.74	1.20
Baltimore, MD area:								
80213	31	8	9	66.11	43.59	78.86	1.52	0.84
80215	31	8	9	87.54	104.60	69.46	0.84	1.26
80215	31	8	11	62.61	98.54	75.41	0.64	0.83
80207	31	8	12	38.53	106.14	64.64	0.36	0.60
80213	31	8	13	587.50	49.23	46.84	11.93	12.54
80215	31	8	14	104.75	84.08	70.50	1.25	1.49
80207	31	8	15	114.19	59.74	59.41	1.91	1.92
80213	31	8	16	434.19	46.57	53.33	9.32	8.14
AVERAGES:				186.93	74.06	64.81	3.47	3.45
Baltimore, MD area:								
80218	31	9	9	92.60	61.84	87.89	1.50	1.05
80203	31	9	10	242.92	68.71	80.65	3.54	3.01
80208	31	9	10	164.27	39.10	93.20	4.20	1.76
80227	31	9	10	149.87	53.54	67.49	2.80	2.22
80201	31	9	10	689.58	104.75	67.77	6.58	10.18
80218	31	9	11	236.96	77.08	104.29	3.07	2.27
80216	31	9	11	56.41	44.33	59.38	1.27	0.95
80201	31	9	12	62.66	57.10	55.75	1.10	1.12
80214	31	9	12	84.25	38.31	45.61	2.20	1.85
80227	31	9	13	44.29	79.83	66.20	0.55	0.67
80216	31	9	14	142.93	30.88	47.70	4.63	3.00
80241	31	9	14	2685.02	47.45	47.40	56.59	56.65
80240	31	9	14	1094.30	59.37	62.87	18.43	17.41
80201	31	9	14	54.42	39.75	35.48	1.37	1.53
80218	31	9	14	134.99	74.27	85.41	1.82	1.58
80208	31	9	15	110.57	45.03	47.08	2.46	2.35
80227	31	9	16	31.56	45.93	61.21	0.69	0.52
AVERAGES:				357.51	56.90	65.61	6.63	6.36

hydrocarbons to the observed NMHC concentration such that the carbon-percent of oxygenates in the observations was equal to the carbon-percent of oxygenates in the predictions. This normalized data set is also presented in Appendix H.

Data taken on different days within the same grid cell were averaged and are presented in Table 7.5 as a summary of the reactivity class analysis. The ratio of the total NMHC in the observed to the predicted data remains in the 4–8 range with lower values in the later time period. The paraffin class constitutes the majority of the NMHC, both in the observations and the predictions. The data indicate that the ROM may slightly overestimate the fraction of carbon represented by this class. It is interesting to note that the carbon-percent of the olefin fraction is consistently overpredicted, although the results for the related class of ethylene are not as clear, with some over- and some underestimates. A few of the afternoon observations show particularly high ethylene fractions. Likewise, the model generally shows an overestimate in the isoprene fraction, although the predictions show that generally less than 1% of the total carbon resides in this class. Concentrations of observed isoprene, when detected, were highly variable. The carbon-percents of the aromatics classes, TOL and XYL, are generally underestimated, except for a few of the afternoon samples where there was little measured aromatic. The carbon-percent of non-reactives shows quite good agreement for the early morning samples between observations and predictions, although the afternoon data show the model to underpredict the carbon-percent.

The reactivity class analysis is useful in that it shows that, despite the obviously large discrepancy between the predicted and observed total NMHC concentrations, there is better correspondence between the fraction of carbon represented by the reactivity classes in the predictions and the observations. This lends further support to the theory of underestimated hydrocarbon emissions as being a primary cause of the concentration underprediction. If there were a fundamental problem in terms of the chemical representation of the reactivity classes we would not expect much correspondence between the predicted and observed carbon fractions. The results shown here support the correctness of the chemical formulation as well as the reactivity splits within the emissions inventory, which are directly reflected in the model results, especially during the early morning period.

Recently there has been much speculation on the role of natural hydrocarbon emissions in O_3 formation. The ROM incorporates two classes of biogenic hydrocarbon in its emissions inventory; isoprene, which is treated explicitly, and the monoterpenes, which are split among the existing reactivity classes. Although no non-urban ambient concentration data exist explicitly for this period that relate directly to the natural hydrocarbons, we present an example of a ROM-generated concentration pattern for isoprene. Figure 7.3 shows the spatial pattern of isoprene concentrations (ppbC) predicted for July 21 at 1500 h. Since isoprene emissions are directly correlated with temperature and solar radiation, this time period should be

TABLE 7.5. SUMMARY OF SELECTED REACTIVITY CLASS PROFILES OF SURFACE NMHC CONCENTRATIONS

Hour (LST)	x	y	NMHC (ppbC) Observed ----> Predicted ---->	%ETH	%OLE	%PAR	%TOL	%XYL	%ISOP	%NONR	%OXY
Obs./Pred. --->											
5--7	28	6	1560.08	6.38	0.95	61.14	8.96	9.51	0.04	4.25	8.77
			189.88	4.74	4.33	64.61	8.06	4.26	0.24	4.98	8.77
			8.22	1.35	0.22	0.95	1.11	2.23	0.17	0.85	1.00
5--7	29	7	952.30	4.03	0.99	55.48	9.66	16.01	0.40	4.95	8.48
			170.28	2.68	5.74	71.56	4.51	2.63	0.79	3.62	8.48
			5.59	1.50	0.17	0.78	2.14	6.08	0.51	1.37	1.00
5--7	30	8	742.95	8.18	1.71	53.46	11.57	12.27	0.00	6.02	6.78
			155.95	3.20	2.66	67.60	8.37	4.48	0.13	6.78	6.78
			4.76	2.55	0.64	0.79	1.38	2.74	0.00	0.89	1.00
5--7	31	8	1043.05	2.17	1.09	63.44	9.21	10.38	0.11	5.88	7.73
			131.76	2.39	1.90	70.57	6.86	3.93	0.07	6.55	7.73
			7.92	0.91	0.57	0.90	1.34	2.64	1.57	0.90	1.00
5--7	39	16	1105.80	6.47	1.23	58.60	11.04	5.69	0.52	8.27	8.18
			137.74	4.78	2.79	66.18	8.32	4.16	0.18	5.41	8.18
			8.03	1.35	0.44	0.89	1.33	1.37	2.89	1.53	1.00
5--7	40	17	596.39	2.67	1.32	59.69	11.06	9.47	0.59	6.50	8.71
			155.84	4.13	2.53	68.79	7.37	3.91	0.03	4.52	8.71
			3.83	0.65	0.52	0.87	1.50	2.42	19.67	1.44	1.00
5--7	52	27	1149.12	3.32	0.32	70.42	8.15	5.08	0.00	4.01	8.70
			156.04	4.16	1.90	69.35	7.14	3.44	0.09	5.22	8.70
			7.36	0.80	0.17	1.02	1.14	1.48	0.00	0.77	1.00
13-13	5	12	129.78	19.62	1.63	37.20	7.34	9.37	0.00	12.98	11.86
			28.96	3.61	2.72	68.83	6.41	2.05	0.25	4.28	11.86
			4.48	5.43	0.60	0.54	1.15	4.57	0.00	3.03	1.00
11-11	29	6	118.11	15.66	1.41	58.19	0.00	0.00	0.00	13.63	11.11
			154.30	3.35	1.58	70.19	5.94	1.70	0.85	5.28	11.11
			0.77	4.67	0.89	0.83	0.00	0.00	0.00	2.58	1.00
15-15	30	7	89.22	2.08	0.47	79.32	3.45	0.00	0.00	5.19	9.48
			58.94	2.05	1.09	72.91	4.67	1.02	1.37	7.41	9.48
			1.51	1.01	0.43	1.09	0.74	0.00	0.00	0.70	1.00

near the maximum for its diurnal emissions pattern. Also, this date was a relatively sunny, hot day across the domain, enhancing the potential for release of isoprene. The figure shows the areas of relatively high values (> 2.5 ppbC) occurring over forested regions, especially in New England. Concentrations of less than 2.5 ppbC are predicted over most of the domain, with maximum concentrations reaching nearly 30 ppbC. Note that contour intervals in the figure are in units of ppm, while the legend indicates the shading interval in units of ppbC. The proper conversion and scaling to a carbon-basis was performed in changing the ppm units which the ROM uses in its computations to the familiar carbon-normalized units of ppbC.

In a review paper, Altshuller (1983) summarizes the available ambient measured isoprene concentration data from various field studies. He shows that a wide range of concentration values exists. Typical average values measured were in the range of 2–4 ppbC in the studies cited, with maximum concentrations in the 20–40 ppbC range. Although the comparison can only be qualitative, the ROM predictions seem to be in the same range as the literature values. Average predicted values in the ROM may be somewhat lower than average observed values, but the subgrid scale problem and the highly reactive nature of isoprene may account for the differences. This comparison lends support for the emission inventory estimates developed for isoprene and for its treatment in the CB-4 chemical mechanism.

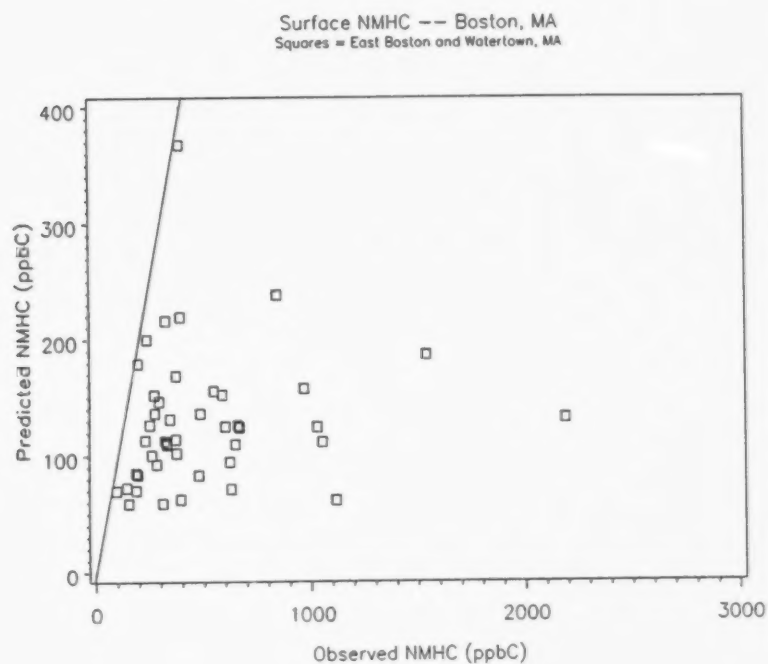
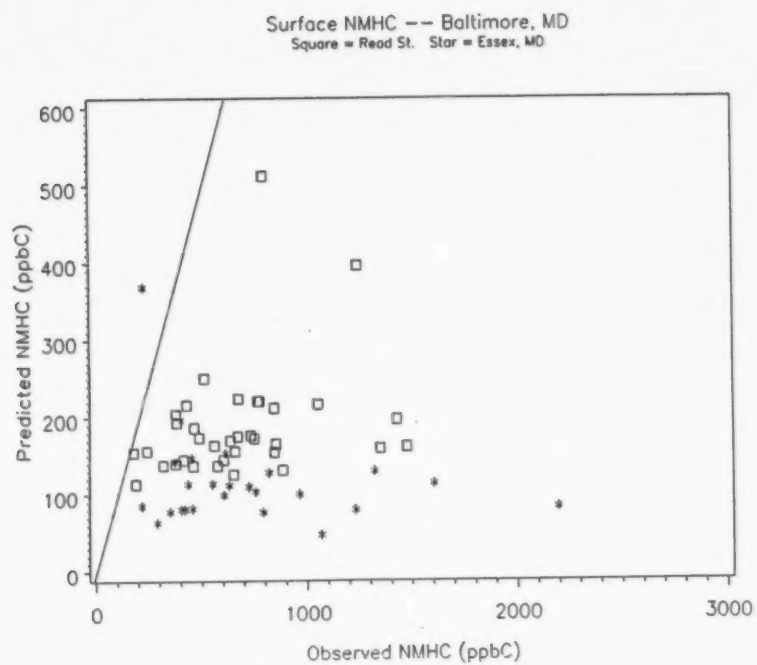


Figure 7.1. Scatterplots of observed (O) and predicted (P1) NMHC data for 06-09 h, LDT by urban area.

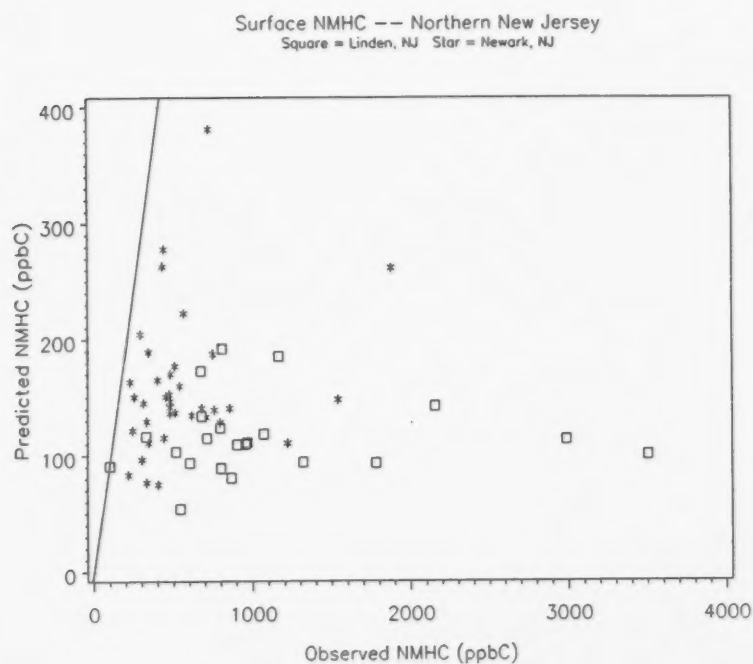
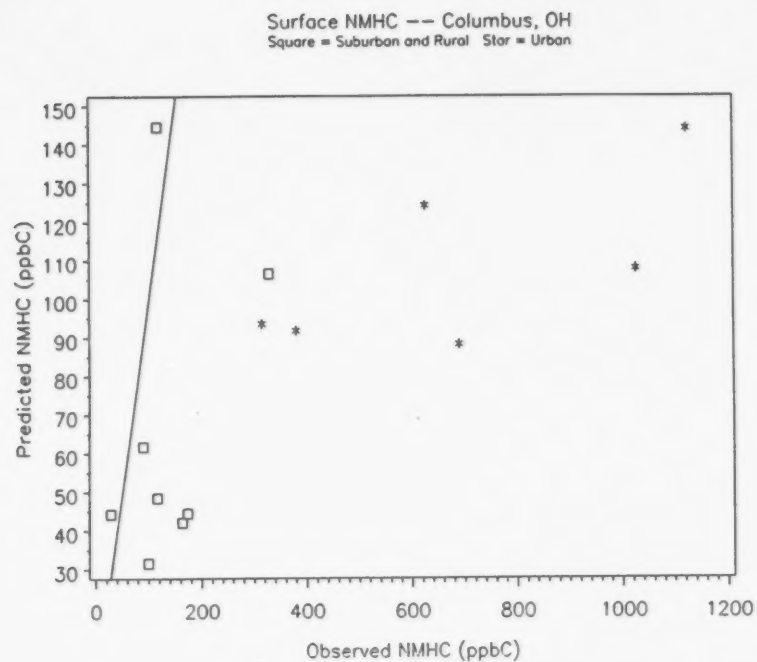


Figure 7.1. (continued)

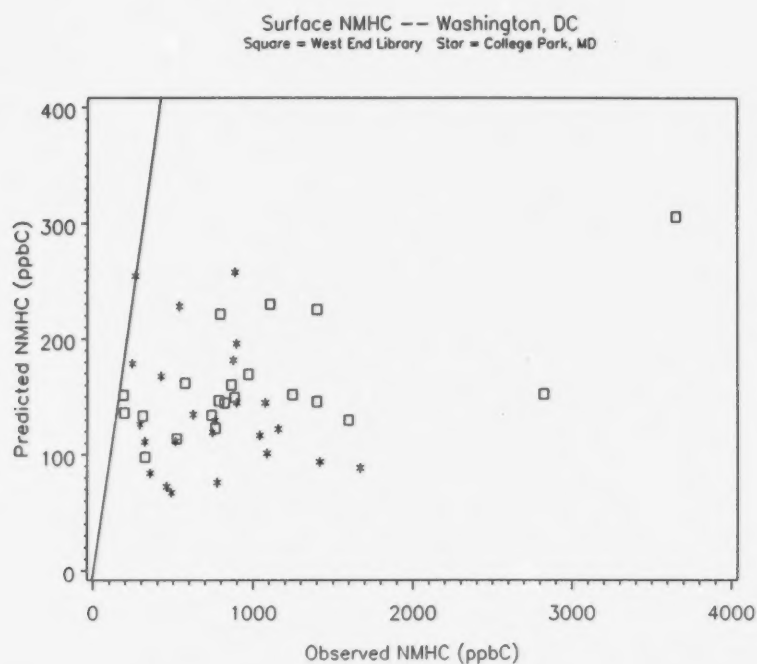


Figure 7.1. (continued)

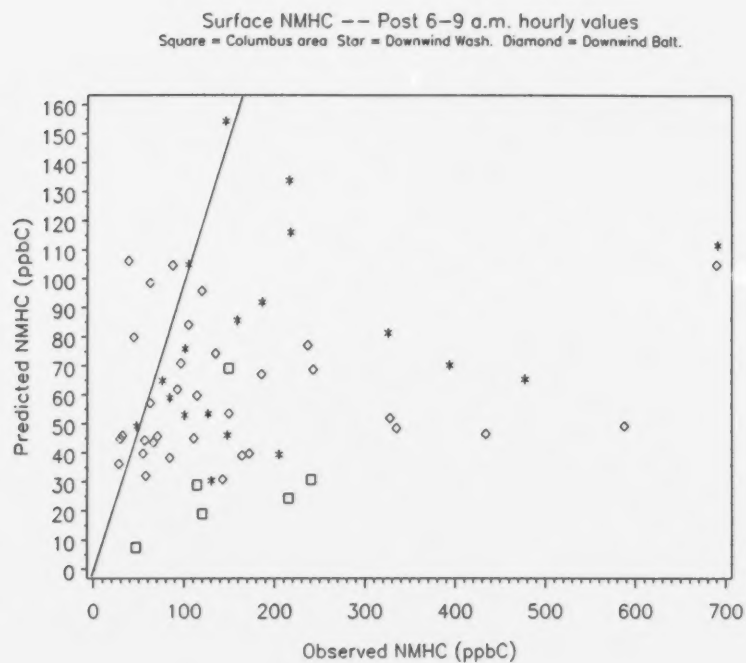


Figure 7.2. Scatterplot of all observed (O) and all predicted (P1) NMHC data for post 06-09 h, LDT period.

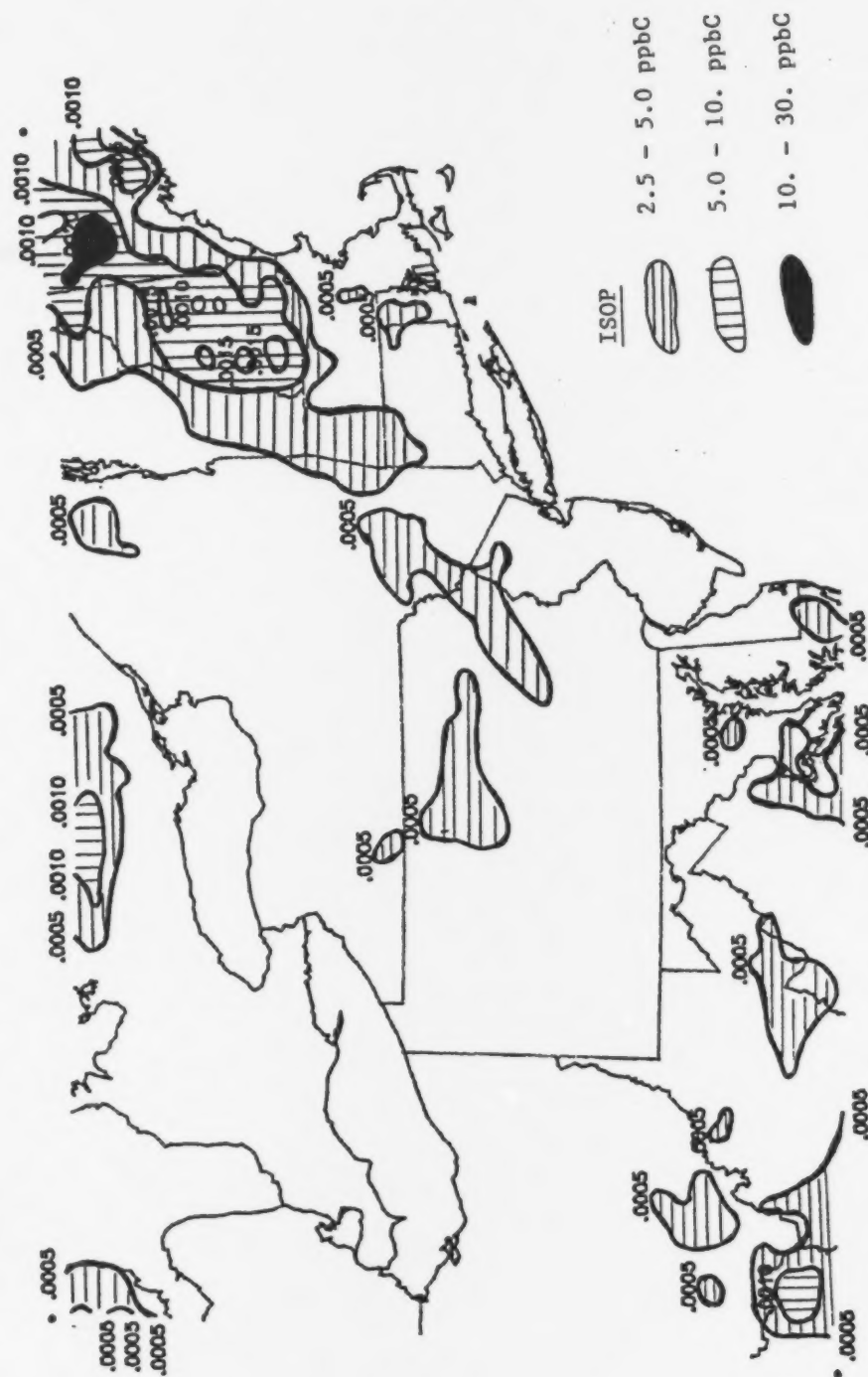


Figure 7.3. Spatial contours of ROM-predicted isoprene concentrations at 1500 h, LST on July 21, 1980. Legend specifies contour interval shadings in units of ppbC; numbers on contours are in units of ppm.

8 EVALUATION WITH AIRCRAFT OBSERVATIONS

8.1 DATA PREPARATION

Several major field programs, including the NEROS, PEPE, and NECRMP, were conducted in the Northeastern U.S. during the summer of 1980. They have been described in an earlier section. As part of these data collection studies, both fixed-wing and helicopter aircraft were used to measure air quality and meteorological parameters above the surface. The 1980 NEROS and PEPE data bases include several long interstate regional flights, urban plume studies near Columbus, OH, and Baltimore, MD, and power plant plume studies in WV. The NECRMP included morning flights upwind and afternoon and evening flights over and downwind of Boston, New York, and Washington, DC. Table 8.1 presents a listing of the aircraft flights analyzed here, the participating agencies, and the availability of O_3 and NO_x data from the flights.¹

Comparison of aircraft data with ROM model results is not a straightforward task. There are some fundamental problems in trying to do this. First, the data sets have different frames of reference. The aircraft is inherently obtaining Lagrangian measurements in a moving frame of reference. Each individual measurement of O_3 or NO_x may represent several seconds of collected ambient air over several hundred meters distance. In contrast, the ROM predictions are hour-integrated concentrations over a volume of space. The ROM's frame of reference is Eulerian, or fixed in space. Because of these differences the analysis we present here is diagnostic rather than quasi-deterministic. Our goal is to provide a general sense of the model's performance at levels above the surface.

¹Most, but not all, flights conducted during the field studies are listed. Flights conducted mostly outside the area of the ROM domain, with a majority of missing data, or with a very localized mission were not included.

TABLE 8.1. SUMMARY OF O₃ and NO_x AIRCRAFT OBSERVATIONS
ANALYZED FROM THE 1980 SUMMER PERIOD

Type of Flight	Location	Agency [†]	Dates (1980)	O ₃	NO _x
Urban	Baltimore	BNL	July 16, 18, 19, 25, 26, 31 Aug. 2, 3, 5, 7, 14	✓	✓
Urban	Baltimore	WSU	July 16, 18, 19, 25, 26, 31 Aug. 2, 3, 5, 7, 8, 14	✓	✓
Urban	Washington	NSI	July 15, 16, 19, 21, 25, 31 Aug. 2, 7, 8	✓	✓
Urban	New York	BNW	July 16, 18, 21, 22, 25, 26, 27, 31 Aug. 2, 4, 5, 6, 7, 8	✓	✓
Urban	Boston	BCL	July 14, 15, 16, 17, 19 Aug. 1, 5, 8, 9	✓	✓
Urban	Columbus	AVNA EMI	July 30, 31 Aug. 4	✓ ✓	✓ ✓
Plume/ Regional	OH→WV	AVNA	July 30	✓	✓
Regional	OH→WV→PA	SRI	July 31	✓	
Regional	OH→PA→NJ	AVNA	Aug.1	✓	✓
Regional	NJ→PA	AVNA	Aug.1	✓	✓
Regional	MI→OH	SRI	Aug.7	✓	
Regional	VT→NY→PA	AVNA	Aug.8	✓	✓
Regional	MD→PA→NJ	AVNA	Aug.8	✓	✓
Regional	OH→MI	AVNA	Aug.15	✓	✓
Regional	MI→OH	AVNA	Aug.15	✓	✓
[†] AVNA=Aerovironment, Inc.; BCL=Battelle Columbus Labs; EMI=Environmental Measurements, Inc.; BNL=Brookhaven National Lab; NSI=Northrop Services, Inc. (U.S. EPA/LV); SRI=Stanford Research Institute; WSU=Washington State Univ.					

The aircraft observations obtained within any given ROM grid cell for a particular flight and a particular hour are integrated to produce a mean concentration.² This mean, along with the standard deviation and the maximum, form the characterized concentration distribution for each hour and grid cell against which the ROM prediction is compared. The prediction's relationship to the mean and standard deviation of the observations provides an indication of the model's performance. Results are presented graphically for O₃ and NO_x.

8.2 RESULTS FOR O₃ and NO_x

8.2.1 Regional Flights

Table 8.1 shows a set of flights performed between July 30 and August 15 that were *regional* in nature. That is, they spanned relatively large areas of the ROM modeling domain. In this section we compare the measurements made for O₃ and NO_x along these flights with ROM predictions. We consider all such flights in this analysis, because they are relatively few in number and they are important for establishing whether the ROM's rural and background predictions are accurate.

The first flight analyzed is an evening flight from July 30 that tracked a plume from Ohio into West Virginia. Figure 8.1 presents the approximate flight path of the aircraft. At selected points along the traverses there is a set of three numbers. The topmost number is the layer of the ROM's vertical structure that corresponds to the aircraft's altitude at that location. The middle number is the observed O₃ value (ppb), and the bottom number is the predicted O₃ value (ppb). The aircraft data have been integrated within each ROM grid cell along the aircraft's flight path; thus, the path shown in Figure 8.1 is an approximation to the true path which is somewhat smoother than that shown. The predicted value is the appropriate hour-averaged O₃ concentration taken from the same grid cell as the integrated observed data. The observations show the aircraft penetrating a plume of relatively high O₃ concentrations, above 80 ppb, with a number of measurements above 100 ppb, at several points along the path. The ROM predictions, however, do not show the same plume. The predicted values are fairly flat in this area, generally around 50 ppb.

Figure 8.2 shows another way of presenting this data. Here we do not see the spatial location of the data points, but we are better able to show all of the aircraft data in one plot. The figure presents data taken at altitudes corresponding to ROM layer 2, approximately 400–1500 m above ground. Within each hour period of the flight, the observed data from each ROM grid cell that the aircraft "flew through"

²Measured concentrations under 5 ppb were considered as missing data because they are in the noise range of the monitors.

are shown as a mean (diamond), with a standard deviation line about the mean value, and a maximum value (diamond) at the top of the concentration distribution. Individual aircraft data were logged at 5–10 s intervals, so there were numerous values entering the mean and standard deviation calculations, depending upon the residence time of the aircraft in any given grid cell. The observed maximum is an instantaneous value. The asterisk represents the ROM prediction from the same hour and grid cell. Within any given hour period shown on the graph there are many grid cells represented, although the cell coordinates are not shown. The sequence of data shown is not necessarily continuous in time, except from hour to hour. Within any hour the data shown are for the grid cells flown through during the hour, but not necessarily in the order in which they were traversed.

The figure shows, in more detail than Figure 8.1, the gap between the predicted and observed concentrations along the aircraft's path. This gap is generally about 30 ppb with greatest differences where the aircraft intersected the plume that it was tracking. Indeed, the maximum O_3 concentrations for July 30 predicted by the ROM in this vicinity show 60–80 ppb values in a plume from the Columbus, OH area during the afternoon along an ESE track from Columbus. At the hours of this particular flight these values are no longer apparent in the predictions in this area.

Figures 8.3 and 8.4 show the corresponding plots for the NO_x data from the same flight. Observed values less than 5 ppb were screened out of the data set, although predicted values less than 5 ppb were not screened out. Therefore, the only meaningful comparisons here are those where the predicted NO_x values are 5 ppb and above. The data show the ROM to be underpredicting NO_x , although the results are not as systematic as they were for O_3 . Both observations and predictions show high values, or spikes, of NO_x corresponding to localized plumes aloft. The locations of these high values are generally not in the same grid cell, although they appear to be in the same general area. The higher values are between 25 and 40 ppb, while the background values observed are 5–10 ppb, and background predicted values are less than 5 ppb.

The next flight considered occurred on July 31 between Columbus, OH and Pittsburgh, PA during the hours of 06–09, LST. The flight was punctuated by occasional rain showers. Several transects were done in the vicinity of Pittsburgh. The geographical display and the time series of O_3 concentrations for the flight are presented in Figures 8.5 and 8.6, respectively. Although no significant plumes were encountered during the flight, the data show a systematic underprediction of the background O_3 concentration along the flight. The observations of O_3 are generally in the 75–85 ppb range while the predictions are in the 45–55 ppb range. No NO_x data were available from this flight.

On August 1 a long-range regional flight was made during the afternoon (13–16 h, LST) from central OH to central NJ. A significant O_3 episode was beginning

along the East Coast at this time. The geographical pattern of the flight, shown in Figure 8.7, shows a gradient in concentrations along the flight, with the highest concentrations in NJ and eastern PA. A gradient can also be seen in the predictions, although its magnitude is not as large. Of course, the diurnal behavior of O_3 also is at work here, so the apparent spatial gradients may not be as large as they seem. The ROM predictions are systematically lower than the observations. This is also apparent in Figure 8.8, the time series from the flight. Note the relatively small standard deviations around the mean observed concentrations. This gives us increased confidence that these observed means are truly regionally representative values. Observed values near the beginning of the flight (OH, western PA) are in the 85–95 ppb range compared to predictions of 50–60 ppb. At the eastern end of the flight observed values had risen to 100–125 ppb with predictions of 60–80 ppb. The ROM has underestimated the regional O_3 background by around 30 ppb as this episode was beginning.

Figures 8.9 and 8.10 show the corresponding NO_x data for this flight on August 1. Observed background values are generally 5–10 ppb, while ROM predictions are generally less than 5 ppb. There is some indication of an increase in NO_x values at the eastern end of the flight in both the observations and the predictions.

Later that day, between 18–19 h, LST, the same aircraft made transects between NJ and north central PA. The geographical and time series plots for O_3 are shown in Figures 8.11 and 8.12, respectively, and those for NO_x are shown in Figures 8.13 and 8.14, respectively. The results here are similar to those for the earlier afternoon flight. Background O_3 concentrations are again underpredicted by 20–30 ppb. Background predicted NO_x concentrations on this flight were more frequently in the 5–10 ppb range (same range as the observed concentrations) than on the earlier flight, although there were still many data values less than 5 ppb.

A north-to-south regional flight was conducted on August 7 from MI (near Detroit) to OH between 18 and 20 h, LST. The flight intersected the urban plume from Detroit about 40 km east of the city. The flight's geographical distribution of O_3 concentrations is shown in Figure 8.15. Mean observed O_3 concentrations near 80 ppb can be seen southeast of Detroit over Lake Erie. These values are 10–15 ppb above the local background, and presumably were sampled in the Detroit urban plume. A local instantaneous maximum of 120 ppb was also seen here, as shown in the corresponding time series for this flight shown in Figure 8.16. Observed values between 80 and 85 ppb were also seen in northern OH during the flight. ROM predictions are generally 20–30 ppb below the observations on this flight. The time series does not clearly show whether there was a predicted plume from Detroit in the area of the aircraft's flight. There is a rise of 10–15 ppb in the predictions from the middle of the flight that may be associated with the remnants of the day's predicted Detroit plume. Contours of maximum predicted O_3 concentrations for this day show an area of 80–100 ppb extending due east from the Detroit area

over Canada and Lake Erie. However, the model may have advected these higher concentrations faster than the actual flow. Hence, by the time of this flight in the early evening the ROM predictions along the flight track did not capture the activity that existed earlier in the day. No NO_x concentrations for this flight were available.

On August 8 a long-range regional flight was conducted from VT to southern PA during 14–17 h, LST. Observed O_3 concentrations at the surface on this day were quite high along the East Coast with maximum afternoon concentrations exceeding 200 ppb in parts of CT and RI. Figures 8.17 and 8.18, respectively, present the geographical and time series data plots of O_3 for this flight. Background observed O_3 values aloft as measured by the aircraft varied from near 100 ppb in PA to 90–95 ppb in southern NY to 70–80 ppb in VT and northern NY. ROM predictions of background O_3 in the same areas were generally 50–60 ppb except toward south-east PA where the ROM's predictions increased to 70–80 ppb, somewhat closer to, although still less than, the observations in this area. Maps of maximum predicted O_3 for this day showed a large area of +80 ppb O_3 values along the immediate East Coast. The southern terminus area of this flight just intersected the edge of the area of higher ROM predicted O_3 concentrations. Observed data at the ground and aloft showed high O_3 concentrations extending farther inland than the ROM predictions.

Figures 8.19 and 8.20 present the geographical and time series plots for NO_x concentrations from the same flight. Background observed concentrations were generally 5–10 ppb over the entire flight, while predicted concentrations were consistently less than 5 ppb. The low predicted values make comparisons with observed NO_x difficult.

The same aircraft performed an evening flight (20–22 h, LST) on August 8 from MD through PA and NJ. The geographical and time series plots of the O_3 data from this flight are presented in Figures 8.21 and 8.22, respectively. During the early portion of the flight over MD and southeast PA the ROM predictions show O_3 values of 70–80 ppb, 10–20 ppb less than the observations. The gap between predictions and observations increases to ≈ 30 ppb over western NJ and eastern PA where observed concentrations were in the range of 90–100 ppb. Then, toward the end of the flight over southern NY, model predictions and observations were in much closer agreement at ≈ 70 ppb. This flight was significant in that it intersected areas of the ROM grid where background grid predictions showed higher excursions over a natural background value.

The corresponding plots for NO_x concentrations of geographical and time series distributions are shown in Figures 8.23 and 8.24, respectively, for this evening flight on August 8. Observed concentrations of NO_x were generally at 8–10 ppb over the entire flight, while ROM predictions of NO_x were again less than 5 ppb.

The last regional flights were conducted on August 15. A mid-day flight (11–13 h, LST) from northern OH to east of Detroit showed relatively low O_3 concentrations. The geographical and time series O_3 plots are shown in Figures 8.25 and 8.26, respectively. The surface air flow was from the north in this area. Observed O_3 concentrations along the flight were in the 50–60 ppb range, as were the O_3 predicted concentrations. Figures 8.27 and 8.28 present the corresponding plots of NO_x concentrations for this flight. Elevated NO_x concentrations were measured by the aircraft to the southeast of the Toledo and Detroit areas as seen in Figure 8.27. Concentrations downwind of Detroit were 20–30 ppb compared to an 8–10 ppb background concentration. The time series plot shows that a sharp NO_x spike in one grid cell near Detroit caused the grid-average to be quite high. ROM predictions of NO_x showed a trend similar to the observations, although they were generally lower. Predicted concentrations of NO_x downwind of Detroit were generally 15–20 ppb; 5–10 ppb lower than the observations.

Later that day (16–19 h, LST) the same aircraft flew from MI to OH making parallel transects along the Lake Erie shorelines. Figures 8.29 and 8.30, respectively, present the geographical and time series plots of O_3 for this flight. Observed concentrations were near tropospheric background levels in the eastern part of the flight path and were just above background for much of the rest of the flight. Elevated concentrations of 75–90 ppb can be seen over Canada east of Detroit and parts of northern OH. ROM predictions follow the observations through most of the flight. There are overpredictions over the northern shore of Lake Erie where the model has developed a larger area of higher concentrations than the aircraft detected, and over eastern OH where the aircraft measured less than 40 ppb O_3 concentrations. Generally, though, the ROM has performed well at predicting concentrations along this flight path.

The geographical and time series plots for NO_x from this flight are shown in Figures 8.31 and 8.32, respectively. Relatively high NO_x concentrations were observed in eastern MI and northern OH on this flight, from 15–30 ppb. Elsewhere, observed NO_x levels were generally 5–10 ppb. The aircraft apparently flew through a few NO_x “plumes” near Detroit leading to some very high localized values. ROM predictions of NO_x along the flight path are often less than 5 ppb, except in southeast MI and along the northwest and southeast Lake Erie shorelines, where predictions were in the 5–10 ppb range. Although the magnitudes of the NO_x predictions are less than the observations, the trend is generally the same.

8.2.2 Urban Flights

As shown in Table 8.1 numerous flights were conducted in the vicinity of urban areas within the Northeast ROM domain during the summer 1980 intensive field

study period, July 12 - August 15. There are too many flights to discuss each one individually here. We have selected 1-4 flights for each individual city that are presented in detail here, including spatial and time series analyses. The selected flights were chosen based on the relatively longer duration of the flight, the data capture rates, and the existing air quality conditions. They are a representative sample from the full collection of flights. The time series plots for those flights not discussed here are presented, without description, in Appendix I. This analysis includes comparison of observed and predicted O_3 and NO_x concentrations from these flights.

The first set of flights considered is that conducted in the Baltimore, MD area as part of the NEROS study (Brown, 1983). Flights conducted on July 16 and 19, and Aug. 2 are reported here.

The Baltimore area was under the influence of a dry high pressure system along the East Coast on July 16. Surface winds were from a SSW direction. Two flights were performed on this day, a morning flight (06-09 h, LST) and an afternoon flight (12-15 h, LST). Figure 8.33 presents the geographical distribution of observed and predicted concentrations along these flights. The flights both roughly follow a pattern including some measurements upwind and over the city, with most measurements taken downwind. The morning flight shows ROM consistently underpredicting O_3 concentrations. Predicted O_3 levels were in the 50-60 ppb range, while observations were generally 80-100 ppb. The afternoon pattern shows ROM O_3 predictions generally of the same magnitude as the observations in the Baltimore area, with some small differences in the spatial location of the O_3 plume. Maximum ROM predictions were in the range of 150-165 ppb, while maximum observations were in the 175-200 ppb range. The time series plots for these flights are shown in Figure 8.34. Here, all data for all grid cells within any one hour of the flight and for each model layer are averaged. Therefore some of the spatial detail in horizontal concentration pattern is lost. Vertical resolution is shown. In an averaged sense, the time series data show the ROM to be underpredicting O_3 in the morning period, and performing quite well in the afternoon period where model predictions are within one standard deviation of the average observations.

The geographical distribution of NO_x concentrations for these flights is shown in Figure 8.35. Observed NO_x values are generally in the range of 15-30 ppb over the area, while predictions are 5-15 ppb directly over the urban area and less than 5 ppb to 10 ppb outside it. The grid-averaged time series for NO_x shown in Figure 8.36 confirms the systematic underprediction during the flights performed on this day. Slightly higher predictions are encountered at the hours the aircraft was closer to the city. The same hours show higher instantaneous maximum concentrations in the observations.

Two flights were also performed on July 19 during the same time periods as the

flights on July 16. Winds were very light and of variable direction over the Baltimore area on this day. Ozone concentrations were generally less than 120 ppb aloft. The geographical distribution for O_3 during these flights is shown in Figure 8.37, and the time series is shown in Figure 8.38. The ROM predictions of 60–95 ppb agree very well with the observations during the morning period. During the afternoon flight, however, observed O_3 values had climbed to the 100–130 ppb range while the predictions had not changed much from the morning values, therefore leading to underpredictions. Contours of maximum O_3 concentrations predicted by the ROM for this day show an area of 100–120 ppb O_3 to the southeast of Baltimore, farther than the aircraft flew on the afternoon transects.

Figures 8.39 and 8.40 present the geographical and time series distributions of NO_x , respectively, from these flights on July 19. Observed and predicted NO_x concentrations were generally quite low on this day in the Baltimore area, often less than 5 ppb. On the morning flight, where significant concentrations of NO_x were occasionally encountered, predictions were in fairly good agreement with observations.

Two flights were conducted in the Baltimore area on Aug. 2, a morning flight from 07–10 h, LST and an afternoon flight from 15–18 h, LST. Winds were light and from the southwest on this day over the Baltimore area. The geographical and time series plots for O_3 from these flights are shown in Figures 8.41 and 8.42, respectively. Agreement between observations and predictions on this day is generally excellent. Maximum afternoon O_3 concentrations were in the 100–120 ppb range in both observations and predictions. Some small differences in spatial location of the highest concentrations can be seen. The light wind speeds on this day, however, could lead to considerable wind field uncertainties.

Geographical distributions and time series of NO_x concentrations for these flights on Aug. 2 are presented in Figures 8.43 and 8.44, respectively. The observed concentration range is generally 5–15 ppb with occasionally higher values, and the predicted NO_x concentrations range is generally 5–10 ppb. Like the O_3 values on this day, the NO_x values are in fairly good agreement for the Baltimore area.

The next set of flights considered occurred in the Columbus, OH and Pittsburgh, PA areas as part of the NEROS field program (Vaughan, 1985). The flights discussed here occurred on July 30 and Aug. 4 near Columbus and on July 31 near Pittsburgh.

On July 30 the Columbus area was on the western side of a large high pressure region. Winds were light and generally from the west. One flight was conducted on this date from 12–16 h, LST. The geographical distribution of O_3 along the flight path is shown in Figure 8.45. Maximum observed concentrations were in the 115–130 ppb range to the southeast of Columbus. Predicted concentrations along

the flight path were generally between 50 and 65 ppb, the same as the background values observed outside of the Columbus urban plume. Apparently the ROM did not produce a significant urban plume in this area during these hours. Contour maps of ROM-predicted maximum O_3 concentrations on this day show an area of 60–80 ppb O_3 to the southeast of Columbus. The timing and location of the flight, however, did not intersect this higher predicted area. Figure 8.46 shows the time series of O_3 for this flight. This figure shows layer 2 values only; each grid cell is shown individually for each hour. The time series substantiates the model's underprediction here. The geographical distribution and time series of NO_x concentrations from this flight on July 30 are presented in Figures 8.47 and 8.48, respectively. ROM predictions of NO_x are generally less than 5 ppb along the flight path, while observations are in the 8–15 ppb range.

Two flights were conducted on Aug. 4 in the Columbus area. The first flight occurred in the afternoon during the period 12–15 h, LST and the second flight occurred in the evening during 19–22 h, LST. A warm front passed through Columbus to the north early on Aug. 4. Winds behind the front were from the south. The geographical and time series plots of O_3 concentrations for these flights are presented in Figures 8.49 and 8.50, respectively. Observed concentrations during the afternoon flight ranged from 58 ppb upwind of Columbus to 100 ppb downwind to 80–90 ppb far downwind in northern OH. Predicted concentrations along this flight track were in the range 50–60 ppb, with little spatial gradient. Most of the evening flight track followed the Lake Erie shoreline in northern OH. Observed concentrations here were generally around 90 ppb, while predictions were consistently in the 50–55 ppb range, although ROM predictions toward the center of Lake Erie on Aug. 4 showed an area of 80–120 ppb O_3 . While individual plumes were not clearly discernible in the observed O_3 concentration data for this day, the general background values of 70–90 ppb were underpredicted by 20–30 ppb.

The geographical and time series plots for NO_x for these flights on Aug. 4 are shown in Figures 8.51 and 8.52, respectively. The observed data appear suspicious in that there is a constant 12 or 13 ppb concentration throughout the flights. Predicted NO_x concentrations are less than 5 ppb throughout, except for the daytime value over Columbus where they are slightly higher.

The final flight discussed in this series occurred on July 31 from 12–13 h, LST using a Columbus-based aircraft. The flight track, however, was a cross-wind transect about 90 km downwind of Pittsburgh. The wind flow was generally westerly to southwesterly, with rain showers in the area. The geographical and time series plots for this flight are shown in Figures 8.53 and 8.54, respectively. The ROM has predicted tropospheric background O_3 values for this area, 40–50 ppb, while the observations show more elevated concentrations. The time series shows plume values reaching as high as 125 ppb for individual grid cell averages. Contours of maximum predicted O_3 values for this day show 40–60 ppb generally over western

PA, with pockets of 60–80 ppb. The extreme southwest corner of the state showed an area of 80–100 ppb. No NO_x concentrations were available from this flight.

The next series of flights discussed occurred in the Boston, MA area as part of the NECRMP field project (Battelle Columbus Labs, 1981). Flights described in detail here took place on July 15 and 16, and August 8, 1980.

During the period of July 15–16 Boston was under the influence of a large "Bermuda" high pressure cell off the East coast, providing south to southwest winds over the area. Considerable transport of O_3 and precursors occurred throughout the Northeast Corridor. Three flights took place on July 15, during the periods of 6–7 h, 10–11 h, and 14–16 h, LST. The morning flights occurred upwind and over the city, while the afternoon flight took place primarily downwind of the city over the ocean. The geographical and time series plots of O_3 concentrations from these flights are presented in Figures 8.55 and 8.56, respectively. The time series plots in Figure 8.56 show all data averaged for all grid cells traversed within any one hour and ROM layer. During the early morning flight the ROM-predicted concentrations show good agreement with the observations as shown by the time series. The geographical displays also show excellent correspondence between observations and predictions. The early morning concentration range was 60–95 ppb, rising to a mid-morning range of 80–125 ppb. In the afternoon downwind flight, the time series shows consistent model underprediction when all grid cells are averaged, but the geographical distribution of concentrations shows that the ROM predictions agree well with the observations immediately to the east and to the southeast of Boston where the O_3 concentrations were generally 140–160 ppb. To the northeast, over the ocean, the model generally predicts O_3 in the 100–130 ppb range while observations are in the 150–165 ppb range.

Contours of maximum predicted O_3 concentrations for this day show Boston to be on the northern edge of a large plume along the East Coast, with highest concentrations over Long Island and CT. While the ROM has developed a plume downwind of Boston, it is not quite as extensive as the observations would suggest, especially to the north and east.

The geographical and time series plots of NO_x concentrations for these flights on July 15 are shown in Figures 8.57 and 8.58, respectively. ROM predictions of NO_x concentrations for the morning flights are generally pretty close to the observations (8–15 ppb), especially for the layer 2 results. During the afternoon flight the ROM has tended to underpredict NO_x , especially to the northeast of Boston. Within the Boston plume, averaged maximum observed concentrations were in the range of 20–30 ppb, while predictions were generally 10–15 ppb. This provides an indication that within an urban plume the model's representation of NO_x is more accurate than under background conditions where more severe underpredictions occurred, as judged by previous flights described.

The next day, July 16, was a continuation of the episode that had developed along the East coast. Wind flow was again from the SW and high O_3 concentrations, in excess of 200 ppb, were observed in southern New England. Three flights were also conducted on this day, from 06–07 h, 10–11 h, and 15–18 h, LST, with the same general flight path patterns as those on July 15. The geographical and time series plots of O_3 concentrations from these flights are shown in Figures 8.59 and 8.60, respectively. The early morning inflow concentrations were generally underpredicted (60–75 ppb predicted vs. 90–100 ppb observed) in layer 2. Data from other layers were fewer and more variable in result. Data from the mid-morning flight showed the ROM to perform quite well for the upwind areas, with 20–25 ppb underpredictions in the near-downwind area where observations were in the 100–110 ppb range. The time series in Figure 8.60 shows the greatest degree of underprediction from the top model layer. The ROM has consistently underpredicted O_3 concentrations along the path of the afternoon flight. Observations downwind of Boston were generally 110–150 ppb, while predictions were in the range 70–100 ppb. The highest observed concentrations occurred south of Boston and over the ocean where the remnants of other combined plumes (New York, Philadelphia) were intercepted. Concentrations of 140–170 ppb were common here. Contours of ROM-predicted O_3 concentrations over the whole domain for this day show the model with a large area of high O_3 values over Long Island, south of the areas with the highest observations. Predicted plume misalignment seems to have been more of a factor on this day than on the previous day.

The geographical and time series analyses for NO_x concentrations for the flights on July 16 are shown in Figures 8.61 and 8.62, respectively. ROM predictions of NO_x (less than 5 ppb) are less than observations (8–10 ppb) during the early morning flight upwind of Boston, with overpredictions over the urban area. For the mid-morning flight the best agreement is over the city (≈ 15 ppb) and near-downwind (9 ppb), while upwind and far-downwind the model predicts less than 5 ppb NO_x values with observations in the 10–15 ppb range. During the afternoon flight the ROM has consistently underpredicted NO_x both upwind and downwind of Boston, again partially due to the plume misalignment occurring on this day.

The final flights discussed in the Boston series occurred on Aug. 8, after the passage of a warm front through the area. Wind flow was from the south and southwest. Three flights were conducted on this day, during the periods 05–07 h, 10–12 h, and 14–16 h, LST. The geographical and time series plots of O_3 concentrations are presented in Figures 8.63 and 8.64, respectively. There is very good agreement between ROM predictions and observations of O_3 along the early morning flight path with concentrations of 50–70 ppb. The mid-morning flight showed 15–30 ppb underpredictions in the downwind area, with better agreement upwind. Some spatial exceptions are noted, but generally the spatial and temporal agreement is good. Most of the afternoon flight occurred over the ocean to the east

of Boston. ROM predictions in the downwind vicinity are fairly accurate, with predictions and observations in the 110–140 ppb range.

Concentrations of NO_x from these flights on Aug. 8 are shown in geographical and time series plots in Figures 8.65 and 8.66, respectively. The time series shows general underprediction by the model. Predictive performance for the morning flights was somewhat better than for the afternoon. Observed morning concentrations of NO_x were in the 8–15 ppb range with predictions in the 5–15 ppb range. On the afternoon flight NO_x concentrations immediately downwind of Boston were observed at ≈ 20 ppb and were predicted at between 4 and 12 ppb. Farther out over the ocean observed concentrations were 14–16 ppb, while ROM predictions were generally in the range of 5–10 ppb.

Aircraft measurements obtained in the New York area will be described next. These measurements were obtained as part of the NECRMP 1980 field studies (Alkezweeny *et al.*, 1981). Flights on July 18, 22, and 25, and on August 8 are discussed.

An upwind morning flight (06–07 h, LST) and a series of afternoon flights (12–19 h, LST) occurred in the New York area on July 18. A cold front passed through the area early on this day. Winds were westerly behind the front, pushing the polluted air mass from the previous days' episode out to sea. The geographical and time series plots of O_3 concentrations from these flights are shown in Figures 8.67 and 8.68, respectively. Concentrations observed on the morning flight in upwind areas over NJ were in the 130–140 ppb range. Model predictions were in the 50–60 ppb range. While the effects of the frontal passage on air quality could be seen clearly in the model predictions here, they were not as apparent from the observations. During the dynamic atmospheric situation of a frontal passage, the timing and location of the front are critical to modeling air quality properly.

An examination of the O_3 concentrations along the afternoon downwind flight paths reveals a sharp gradient in concentrations from the northwest to the southeast, following the path of the cold front's movement. Predicted concentrations are in general agreement with observations here, although there are some spatial disparities. The highest predicted concentrations along the flight path are 140–150 ppb, while observations in one small area south of Long Island were 200–230 ppb. These higher concentrations may have been remnants of the episode occurring over the previous several days.

The geographical and time series plots of NO_x concentrations from the flights on July 18 are shown in Figures 8.69 and 8.70, respectively. Observed concentrations from the morning flight were mostly erroneous and are not shown. Predicted concentrations along the downwind flight track agree fairly well with observations. The time series shows the model to be underpredicting, but the predicted concentra-

tions are well within the standard deviation of the observations. ROM predictions of 15–20 ppb NO_x were common through the area, with observations only slightly higher including maximum values of 35–40 ppb.

The New York area was in the midst of another significant episode on July 22. A Bermuda high pressure region off the Atlantic coast was creating strong SW flow along the Northeast Corridor, providing significant interurban transport of O_3 and precursors. Flights were made in the morning (06–07 h, LST) over upwind areas and in the afternoon (12–18 h, LST) over downwind areas. The geographical and time series plots of O_3 concentrations along the flight paths are shown in Figures 8.71 and 8.72, respectively. ROM performance for O_3 on this day is excellent. Predicted and observed concentrations for the early morning upwind flight are nearly identical, between 65 and 75 ppb. Predicted concentrations for the later flight show a significant O_3 plume emanating to the northeast from the NY area with maximum concentrations of 150–170 ppb. Maximum observed concentrations range from 180–250 ppb in the same area. An examination of contours of the maximum predicted O_3 values for this day over the ROM domain shows a strong plume centered over central CT with a SW–NE axis. Judging from air quality observations from aircraft and surface monitors the predicted placement of the NY plume for this day is very accurate. This lends support to the observation that when transport calculations and plume placement are not biased in the model's results, air quality predictions for O_3 are most accurate.

The geographical and time series plots for NO_x from the flights on July 22 are shown in Figures 8.73 and 8.74, respectively. The time series indicates that the ROM results underpredict NO_x concentrations, especially for layer 1, where some of the higher observed concentrations are located. The spatial plot, in Figure 8.73, shows that, for layer 2, the model predictions within the NY plume are in the 20–25 ppb range, while the observations within the plume are in the 30–50 ppb range. Outside of this central plume area, predictions and observations are fairly close.

On July 25 an upwind morning flight (06–07 h, LST) and a series of downwind afternoon flights (12–18 h, LST) were made in the New York area. A dry high pressure system was centered directly over the area, with light and variable winds at the surface. The geographical and time series plots of O_3 concentrations along these flight paths are shown in Figures 8.75 and 8.76, respectively. For this day the ROM again performs very accurately at developing an O_3 plume downwind from NY. Comparison of results from the upwind morning flight shows ROM-predicted concentrations of 44–47 ppb and observations from 43–76 ppb. The downwind afternoon flight shows good agreement between predictions and observations, with the core of the ROM-predicted O_3 plume located 20–40 km south of the observed plume. The time series plot shows ROM predictions generally consistently fall within the standard deviations of the observations for the average over grid cells within an hour. The spatial plot showing layer 2 concentration distributions also

shows that maximum O_3 values in the observations and predictions fall in the 140–150 ppb range, with some small differences in spatial location.

Concentrations of NO_x from the flights on July 25 are shown in geographical and time series plots in Figures 8.77 and 8.78, respectively. Model predictive performance for NO_x for these flights is excellent, especially for the downwind within-plume concentrations. Highest predicted and observed NO_x concentrations for the afternoon flight were in the 25–30 ppb range. Some small differences in the spatial location of the maximum concentration areas are noted, but these are expected considering the variable nature of the winds on this day.

On Aug. 8 an upwind morning flight (06–07 h, LST) and a downwind afternoon flight (12–15 h, LST) were conducted in the NY area. A strong high pressure cell was centered over the middle Atlantic states providing strong westerly to southwesterly flow through the NY area. Observed O_3 concentrations from 200 to 250 ppb were seen at the surface and aloft downwind over CT on this day. The geographical and time series analyses of O_3 concentrations for these flights are presented in Figures 8.79 and 8.80, respectively. The figures show that the observed morning upwind concentrations of 70–90 ppb are underpredicted by 10 to 20 ppb. Spatial results for the afternoon downwind flight, shown in Figure 8.79, show that the NY plume developed by the model is somewhat south of that as defined by the observations. Maximum predictions are in the range of 160–170 ppb over Long Island sound and eastern Long Island, while maximum observations are 200–250 ppb over southeast CT. Over central CT, predictions drop off to 70–90 ppb levels with observations generally all at +125 ppb levels. The time series of results shows general underprediction for the afternoon flight, although the predicted O_3 values lie just outside the envelope defined by the standard deviation.

The geographical and time series plots for NO_x concentrations from the flights on Aug. 8 are shown in Figures 8.81 and 8.82, respectively. Maximum NO_x concentrations predicted in the afternoon downwind plume are on the order of 25–30 ppb, comparing favorably with the observed values of 30–40 ppb. The spatial extent of the higher concentrations, though, is much larger in the observed field of concentrations. The integrated result, as shown by the time series in Figure 8.82, indicates general underpredictions along the afternoon flight path. ROM predictions of 10–20 ppb were common through the extent of the predicted plume, while observations of 15–30 ppb were the rule through the observed plume area.

The final series of aircraft flights discussed took place in the Washington, DC area during the NECRMP 1980 field studies (Wengert and Rutherford, 1981). The specific flights described occurred on July 15, 21, and 25.

The Washington area was under the influence of a strong dry high pressure system located off the East coast on July 15. Winds near the surface were from

the south and southwest. Two series of flights were made, a morning upwind series (05–10 h, LST) and an afternoon downwind series (13–16 h, LST). The geographical and time series plots for O_3 concentrations from these flights are presented in Figures 8.83 and 8.84, respectively. The figures show that the ROM underpredicted O_3 concentrations during the morning flight. Predicted concentrations were in the range of 40–55 ppb, while observed concentrations were 75–85 ppb. The time series, in Figure 8.84, shows that the underpredictions from layer 2 are slightly greater than those from either layers 1 or 3. Afternoon flights to the east and northeast of Washington showed observed O_3 levels of 100–115 ppb at downwind locations with predicted levels of 80–92 ppb. The time series shows that, for the afternoon flights, the degree of underprediction is worst for layer 1, and somewhat less for layers 2 and 3. Contours of maximum predicted O_3 concentrations for this day show a strong O_3 plume emanating from the Baltimore area, with concentrations as high as 160 ppb. For the nearby Washington area, however, there does not appear to be a discernible plume developed.

The geographical and time series plots for NO_x concentrations from these flights are presented in Figures 8.85 and 8.86, respectively. Predicted concentrations are generally less than 5 ppb, while observed NO_x concentrations are in the range 5–10 ppb. The time series shows that predictions and observations have the same trend, but that observed concentrations are subject to extreme instantaneous values, affecting the grid-hour average.

July 21 occurred in the middle of a significant East coast O_3 episode affecting the Washington area as well as other Northeast U.S. cities. Wind flow was weak and generally from the SW as the off-shore high pressure system became stagnant. Two flights were conducted in the Washington area on July 21, a morning flight (05–10 h, LST) and an afternoon flight (13–15 h, LST). The geographical and time series plots of O_3 concentrations from these flights are shown in Figures 8.87 and 8.88, respectively. Model predictions from the morning flight were in a tropospheric background range of 45–50 ppb over most of the flight path, except for the immediate Washington area where 70–75 ppb O_3 was predicted. Observed O_3 concentrations for this flight were 65–75 ppb with some values in the 80–85 ppb range downwind of Washington. It is obvious here that the regional background O_3 concentrations affecting the Washington area were underpredicted by the ROM. Afternoon concentrations of observed O_3 were ≈ 120 ppb downwind of Washington, and 160–190 ppb near the Baltimore area. Model predictions were 60–80 ppb and 80–85 ppb in the same respective areas. Contours of ROM-predicted maximum O_3 concentrations for July 21 show a small urban plume of 80–100 ppb values centered over Washington, much reduced in size and concentration magnitude from the actual plume as judged from aircraft and surface O_3 measurements.

The geographical and time series plots of NO_x concentrations from these flights on July 21 are shown in Figures 8.89 and 8.90, respectively. Predicted concentra-

tions of NO_x along the flight paths are generally less than 5 ppb, except for the morning flight over the immediate metropolitan area where concentrations of 10–20 ppb were encountered. Observed NO_x values were generally 5–10 ppb during the flights, again except for the morning flight near the urban area where ≈ 40 ppb values were encountered. The time series, in Figure 8.90, echoes these underpredictions, but also indicates that the model performance for the morning flight was often within the uncertainty band of the measurements as defined by the standard deviation.

On July 25 a large high pressure system was centered over the middle Atlantic states, providing light and variable winds in the Washington area. Two series of flights were conducted on this day, a morning upwind series (04–06 h, LST) and a late morning-afternoon series (09–15 h, LST). The geographical and time series plots of O_3 concentrations from the early morning flights are shown in Figures 8.91 and 8.92, respectively. During the morning flight, both the observations and predictions of O_3 concentrations were in the range of 45–55 ppb. During the afternoon flights there is also good agreement between observations and predictions. In the immediate Washington area observed and predicted concentrations were in the 65–75 ppb range with 75–115 ppb values to the east of the city. The flights also took the aircraft downwind of Baltimore where observed and predicted concentrations were in the 90–120 ppb range. The time series, shown in Figure 8.92, reflects the excellent model performance for O_3 on July 25.

The geographical and time series plots of NO_x concentrations from the flights on July 25 are shown in Figures 8.93 and 8.94, respectively. Observed and predicted concentrations during the morning flight were frequently less than 5 ppb. In the immediate Washington area, 6–7 ppb NO_x concentrations were seen in both observations and predictions. During the afternoon flights, particularly high concentrations of NO_x were observed to the east and northeast of Washington. Observed maximum values here were in the range of 30–60 ppb, with predictions of 10–20 ppb in the same area. Outside of this maximum area, agreement between observed and predicted concentrations is generally good. This is also shown in the time series in Figure 8.94, especially in layer 2 where the agreement is best.

8.3 RESULTS FOR NMHC

Grab samples of air were obtained during most of the flights listed in Table 8.1 for subsequent hydrocarbon analysis. Typically, 2–4 samples were obtained intermittently during a flight at different locations. Unlike the surface hydrocarbon samples which were obtained over a one-hour period at one location, the aircraft samples were obtained over a period of several minutes of flight time. The processing of the samples by subsequent chromatographic analysis proceeded in the same

manner as previously described in Section 7 for the surface hydrocarbon samples.

The earlier caveats concerning hydrocarbon data also apply here; principally, the sporadic nature of the measurements and the lack of oxygenated organic data from the observations. There are different problems with the representativeness of the aircraft hydrocarbon data than there are with the surface data. The surface data were apt to show very localized influences because of siting constraints, although the temporal aspects of the measurements were on the same scales as the ROM output. Conversely, the aircraft hydrocarbon measurements are more spatially representative than the surface measurements because they are obtained over a broader area and are farther from direct source influences, although the temporal scale of the measurements is much shorter than the 1-hr time scale of the ROM output. For these reasons we present the comparison of observed and predicted NMHC data in a deterministic manner for diagnostic purposes.

The data are aggregated according to location, rather than specific flight. For example, Table 8.2 presents all of the aircraft NMHC data available for the Baltimore area for the summer 1980 period. For a particular flight and time period the data are averaged. The data are also averaged for altitudes within ROM layers 1 and 2 together, while layer 3 data are kept separate. ROM grid cell location data are not shown because the aircraft sampled in different locations over the Baltimore area. For any given time period, samples may have been obtained in locations corresponding to different ROM grid cells. For a given sample, predicted data were chosen from the same ROM grid cell as the location of the sample. Entries in Table 8.2 showing multiple samples therefore most likely have data averaged from different grid cells within the general Baltimore area.

The table shows, for each date and time period, the number of samples that were obtained (N) and the ROM layers corresponding to the altitudes at which the samples were obtained. The observed and predicted values of NMHC are shown along with their ratio (O/P). As was the case with the surface data, two methods of obtaining the predicted data were used. The strictly matched predicted data, P1, were obtained from the same grid cell as the location of the observed data. The predicted P2 data were obtained from the 9-cell average centered on the grid cell used to obtain P1. P2 represents a broader spatial prediction corresponding to a more quasi-deterministic match of observed and predicted data. We generally see only slightly lower values in P2 compared to P1 in the analyses to follow. We will discuss the results for comparisons of observed and predicted P1 data, although the results for P1 also apply to P2.

Table 8.2 shows that the average observed NMHC concentration from the aircraft samples over the Baltimore area was 79.2 ppbC during the summer 1980 period. This compares with a corresponding predicted value of 55.8 ppbC, with a ratio of observed to predicted of 1.67. For comparison, the surface NMHC data

TABLE 8.2. SUMMARY OF NMHC CONCENTRATIONS, OBSERVED AND PREDICTED, ALOFT OVER THE BALTIMORE AREA DURING THE 1980 SUMMER PERIOD.

DATE	LOCATION	ROM LAYERS	N TIME PERIOD (hr, LST)	NMHC(O) (ppbC)	NMHC(P1) (ppbC)	NMHC(P2) (ppbC)	O/P1 RATIO	O/P2 RATIO
80197	Baltimore Area	2	5 9-10	42.446	74.062	65.214	0.573	0.651
80197	Baltimore Area	2	2 9- 9	206.180	66.303	61.955	3.110	3.328
80197	Baltimore Area	1 2	4 12-13	75.835	51.820	52.428	1.463	1.446
80198	Baltimore Area	2	1 6- 6	196.310	26.646	44.430	7.367	4.418
80198	Baltimore Area	2	3 8- 9	149.503	63.770	63.193	2.344	2.366
80198	Baltimore Area	2	2 9-11	18.275	57.947	61.850	0.315	0.295
80198	Baltimore Area	2	3 13-15	227.507	73.049	79.740	3.114	2.853
80198	Baltimore Area	2	3 14-15	62.880	90.255	79.703	0.697	0.789
80200	Baltimore Area	1 2	2 7- 7	84.005	106.090	73.275	0.792	1.146
80200	Baltimore Area	2	3 8- 9	25.307	46.254	56.243	0.547	0.450
80200	Baltimore Area	2	3 13-15	117.773	46.457	39.270	2.535	2.999
80201	Baltimore Area	1 2	3 7- 8	264.917	73.173	80.027	3.620	3.310
80201	Baltimore Area	2	2 8- 9	30.695	46.985	54.630	0.653	0.562
80201	Baltimore Area	2	3 10-10	37.980	99.186	74.210	0.383	0.512
80201	Baltimore Area	2	2 13-13	254.080	42.585	40.345	5.966	6.298
80201	Baltimore Area	2	3 15-15	72.290	32.639	33.980	2.215	2.127
80203	Baltimore Area	2	4 8- 9	30.640	71.380	73.053	0.429	0.419
80203	Baltimore Area	2	4 9-11	5.050	59.965	64.980	1.418	1.309
80203	Baltimore Area	2	2 10-11	76.615	59.928	63.025	1.278	1.216
80203	Baltimore Area	1 2	5 16-17	36.450	38.856	38.064	0.938	0.958
80206	Baltimore Area	2	3 9-10	67.537	82.900	52.177	0.815	1.294
80206	Baltimore Area	3	1 10-10	13.700	3.046	3.280	4.497	4.177
80206	D.C.-Maryland	2	4 15-16	44.338	36.753	32.913	1.206	1.347
80206	Baltimore Area	2	4 17-17	81.218	28.566	29.350	2.843	2.767
80207	Baltimore Area	2	5 8-10	184.504	69.096	57.334	2.670	3.218
80207	Baltimore Area	2	4 11-12	79.412	90.698	58.362	0.876	1.361
80207	Baltimore Area	2	5 15-16	51.680	52.698	47.644	0.981	1.085
80208	Baltimore Area	2	4 10-11	137.262	26.795	33.173	5.123	4.138
80208	Baltimore Area	2	1 10-10	18.500	34.465	38.310	0.537	0.483
80208	Baltimore Area	2	4 13-15	44.133	31.988	32.235	1.380	1.369
80209	Baltimore Area	2	1 9- 9	46.940	58.782	54.560	0.799	0.860
80209	Baltimore Area	2	5 11-12	39.140	46.514	37.812	0.841	1.035
80209	Baltimore Area	1 2	4 15-18	46.270	40.514	38.195	1.142	1.211
80213	Baltimore Area	2	4 13-14	66.903	49.286	40.520	1.357	1.651
80213	Baltimore Area	2	4 14-15	79.175	51.656	42.120	1.533	1.880
80214	Baltimore Area	2	3 12-14	76.817	41.623	36.007	1.846	2.133
80215	Baltimore Area	2	3 9-10	69.573	74.296	57.043	0.936	1.220
80215	Baltimore Area	2	3 11-13	65.153	59.111	51.107	1.102	1.275
80215	Baltimore Area	2	4 15-16	92.740	70.291	63.470	1.319	1.461
80215	Baltimore Area	2	4 18-18	44.013	81.501	77.613	0.540	0.567
80216	Baltimore Area	2	5 12-13	66.372	44.618	47.642	1.488	1.393
80218	Baltimore Area	2	2 8- 9	51.205	58.573	76.125	0.874	0.673
80218	Baltimore Area	2	3 13-15	89.863	76.476	70.687	1.175	1.271
80218	Baltimore Area	2	3 14-15	39.463	41.508	49.280	0.951	0.801
80219	Baltimore Area	2	3 7- 8	39.707	143.062	77.650	0.278	0.511
80219	Baltimore Area	2	3 10-10	89.010	59.188	53.183	1.504	1.674
80219	Baltimore Area	2	4 13-14	68.760	41.930	37.755	1.640	1.821
80219	Baltimore Area	1 2	4 15-17	55.513	37.023	35.875	1.499	1.547
80220	Baltimore Area	2	4 9-11	33.392	43.997	59.103	0.759	0.565
80220	Baltimore Area	2	3 12-13	71.923	62.178	60.000	1.157	1.199
80227	Baltimore Area	2	3 12-12	35.873	25.988	33.170	1.380	1.081
80227	Baltimore Area	2	1 19-19	62.770	34.900	37.390	1.799	1.679
80228	Baltimore Area	2	1 1- 1	50.540	28.886	27.540	1.750	1.835
AVERAGES:				79.210	55.778	51.854	1.667	1.661

analyzed for Baltimore, shown in Section 7, contained an average observed value of 643 ppbC for the grid cells in the Baltimore area with a corresponding predicted value of 143.1 ppbC, and a ratio of 5.5. The observed values aloft are obviously lower and less locally influenced than the early morning surface values. The model still shows an average underprediction here for NMHC, but an examination of the individual data in Table 8.2 shows that it is not systematic. There are numerous overpredictions scattered among the data. A comparison of the surface-collected observed data to the aircraft data shows that a large vertical gradient of NMHC exists. There is as much as a ten-fold decrease from the surface to aloft. Of course, most of the surface data were collected during the early morning traffic period, and the aircraft data were obtained later in the morning and afternoon. This, however, probably does not account for all of the difference. For the Baltimore area, the averaged predicted value of NMHC used in the aircraft analysis is about three times lower than the average predicted value from the surface analysis. The time difference probably does account for most of this predicted concentration variation.

Tables 8.3, 8.4, and 8.5 show the corresponding data for the Washington, New York, and Boston urban areas. The results are fairly similar to those found for Baltimore, except for the Washington area. Average observed NMHC concentrations over the summer period were 182.2, 75.0, and 62.4 ppbC for the Washington, New York and Boston areas, respectively. Average predicted NMHC values for these areas were 76.0, 63.4, and 65.3 ppbC, respectively, with O/P ratios of 2.8, 1.4, and 1.1. The higher value of observed NMHC aloft over Washington may be an artifact of the aircraft in that the helicopter used in the Washington study was able to sample at lower altitudes than the fixed wing aircraft used for the other cities.³ The large vertical gradients that appear in the observed NMHC data give rise to higher concentration values the closer to the surface the aircraft is able to fly. In all cases the aircraft data are considerably lower in concentrations than the surface values for the urban areas. Also, except for Washington, the underprediction does not appear to be systematic aloft.

Aircraft samples were also obtained in non-urban areas during regional flights and over eastern Ohio during plume studies out of Columbus.⁴ Three broad geographic areas were defined for aggregating hydrocarbon samples: NY-VT, PA-MD, and eastern OH. The NMHC results for these areas are shown in Table 8.6. Results for the first two areas, which contain most of the rural samples, are strikingly similar. Average observed and predicted NMHC concentrations were about 38 and 27 ppbC respectively, approximately a 30% underprediction, for both areas. The observed and predicted levels for both areas were considerably less than those obtained

³The helicopter used for the Washington sampling was able to conduct spirals very low over the Potomac River. In other cities, particularly New York City, the aircraft had to remain further from the downtown area and at a higher altitude.

⁴While Columbus is not a rural area, the NMHC concentrations obtained from samples in the Columbus area were combined with others from more rural downwind areas of eastern Ohio.

TABLE 8.3. SUMMARY OF NMHC CONCENTRATIONS, OBSERVED AND PREDICTED, ALOFT OVER THE WASHINGTON AREA DURING THE 1980 SUMMER PERIOD.

DATE	LOCATION	FROM LAYERS	N	TIME PERIOD (hr, LST)	NMHC(O) (ppbC)	NMHC(P1) (ppbC)	NMHC(P2) (ppbC)	O/P1 RATIO	O/P2 RATIO
80198	Washington Area	1	1	7- 7	386.930	75.779	90.380	5.106	4.281
80201	Washington Area	2	2	9-10	285.760	98.073	58.910	2.914	4.851
80203	Washington Area	1 2	2	6- 7	41.140	105.778	107.650	0.389	0.382
80207	Washington Area	2	2	5- 6	32.590	15.002	17.480	2.172	1.864
80213	Washington Area	1 2	2	7- 8	213.445	28.865	29.610	7.395	7.209
80213	Washington Area	2	1	9- 9	315.250	141.610	65.440	2.226	4.817
80214	Washington Area	1 2	2	5- 5	163.465	89.580	94.745	1.825	1.725
80215	Washington Area	1 2	2	5- 6	146.080	56.754	79.225	2.574	1.844
80220	Washington Area	1 2	4	7- 9	183.145	97.729	79.778	1.874	2.296
80221	Washington Area	1 2	3	8- 9	97.640	47.653	60.993	2.049	1.601
80222	Washington Area	1 2	3	5- 7	138.570	79.165	66.667	1.750	2.079
AVERAGES:					182.183	75.999	68.262	2.752	2.995

TABLE 8.4. SUMMARY OF NMHC CONCENTRATIONS, OBSERVED AND PREDICTED, ALOFT OVER THE NEW YORK AREA DURING THE 1980 SUMMER PERIOD.

DATE	LOCATION	FROM LAYERS	N	TIME PERIOD (hr, LST)	NMHC(O) (ppbC)	NMHC(P1) (ppbC)	NMHC(P2) (ppbC)	O/P1 RATIO	O/P2 RATIO
80198	New York Area	2	1	6- 6	61.960	75.359	63.180	0.822	0.981
80198	New York Area	2	1	6- 6	50.130	75.359	63.180	0.665	0.793
80198	New York Area	2	1	7- 7	56.020	45.464	62.060	1.232	0.903
80200	New York Area	1 2	3	5- 6	19.020	41.545	40.153	0.458	0.474
80201	New York Area	1 2	4	5- 6	142.587	53.922	56.485	2.644	2.524
80203	New York Area	1 2	3	5- 6	98.787	86.137	93.667	1.147	1.055
80204	New York Area	1 2	3	5- 6	129.970	64.397	81.000	2.018	1.605
80204	New York Area	1	1	17-17	120.990	141.810	139.540	0.853	0.867
80206	New York Area	1 2	2	5- 6	16.380	41.504	38.775	0.395	0.422
80207	New York Area	2	2	5- 5	45.850	10.502	12.100	4.366	3.789
80210	New York Area	1 2	2	7- 7	89.260	23.511	18.870	3.796	4.730
80213	New York Area	1 2	2	5- 6	32.930	39.242	38.360	0.839	0.858
80213	New York Area	1	1	17-17	117.150	97.846	87.170	1.197	1.344
80215	New York Area	1 2	3	5- 6	52.370	53.233	50.083	0.984	1.046
80218	New York Area	1 2	2	6- 6	165.950	155.758	145.735	1.065	1.139
80219	N.Y.-N.J. Area	2	1	0- 0	34.100	31.559	29.660	1.081	1.150
80219	New York Area	1 2	3	5- 6	83.957	98.695	108.477	0.851	0.774
80220	New York Area	1	1	9- 9	67.080	55.598	88.620	1.207	0.757
80221	New York Area	2	2	5- 6	71.150	32.444	36.860	2.193	1.930
80221	New York Area	1	1	13-13	45.200	44.960	45.520	1.005	0.993
AVERAGES:					75.042	63.442	64.975	1.441	1.407

TABLE 8.5. SUMMARY OF NMHC CONCENTRATIONS, OBSERVED AND PREDICTED, ALOFT OVER THE BOSTON AREA DURING THE 1980 SUMMER PERIOD.

DATE	LOCATION	ROM LAYERS	N	TIME PERIOD (hr, LST)	NMHC(O) (ppbc)	NMHC(P1) (ppbc)	NMHC(P2) (ppbc)	O/P1 RATIO	O/P2 RATIO
80196	Boston Area	1	2	5-7	60.015	82.939	81.435	0.724	0.737
80196	Boston Area	1 2	2	9-10	63.545	89.965	78.605	0.706	0.808
80196	Boston Area	3	1	10-10	74.970	20.539	16.700	3.650	4.489
80196	Boston Area	2	1	15-15	48.040	55.620	58.640	0.864	0.819
80197	Boston Area	1 3	3	5-6	31.187	50.556	56.683	0.617	0.550
80197	Boston Area	1 2	2	9-9	130.190	69.257	77.575	1.880	1.678
80197	Boston Area	3	2	9-9	18.035	44.581	43.470	0.405	0.415
80197	Boston Area	2	1	15-15	153.000	73.485	75.120	2.082	2.037
80198	Boston Area	1	1	5-5	83.890	293.188	280.610	0.286	0.299
80198	Boston Area	2	2	6-6	51.910	41.491	48.280	1.251	1.075
80198	Boston Area	1 2	3	9-10	81.010	93.704	100.440	0.865	0.807
80198	Boston Area	2	1	15-15	50.990	42.526	45.870	1.199	1.112
80198	Boston Area	2	1	17-17	124.020	42.269	46.480	2.934	2.668
80199	Boston Area	3	1	6-6	45.010	26.471	31.190	1.700	1.443
80199	Boston Area	2	1	6-6	23.880	49.193	58.420	0.485	0.409
80199	Boston Area	2	2	9-10	128.425	96.670	88.515	1.328	1.451
80199	Boston Area	2	1	16-16	68.970	58.206	58.060	1.185	1.188
80201	Boston Area	1 2	3	5-6	27.997	53.930	56.953	0.519	0.492
80201	Boston Area	2	2	9-10	45.955	48.828	47.075	0.941	0.976
80201	Boston Area	2	1	13-13	42.960	31.494	28.200	1.364	1.523
80206	Boston Area	1	1	6-6	38.000	67.398	61.530	0.564	0.618
80206	Boston Area	1 2	2	9-10	56.450	108.723	87.820	0.519	0.643
80207	Boston Area	1 2	2	5-6	20.505	40.749	41.735	0.503	0.491
80207	Boston Area	2	3	9-10	32.543	102.251	71.510	0.318	0.455
80213	Boston Area	1 2	3	5-6	40.350	42.849	41.290	0.942	0.977
80213	Boston Area	1 2	2	9-10	121.410	63.331	64.265	1.917	1.889
80214	Boston Area	2	3	5-5	36.940	43.686	45.133	0.846	0.818
80214	Boston Area	2	4	8-9	81.023	54.030	57.665	1.500	1.405
80218	Boston Area	1 2	3	5-6	93.247	77.072	68.057	1.210	1.370
80218	Boston Area	1 2	4	9-10	188.758	154.893	107.460	1.219	1.757
80218	Boston Area	2	1	20-20	16.130	66.366	76.950	0.243	0.210
80221	Boston Area	1 2	3	5-6	31.300	79.881	79.400	0.392	0.394
80221	Boston Area	1 2	2	9-10	109.870	98.765	93.750	1.112	1.172
80222	Boston Area	1	1	5-5	90.010	58.752	92.050	1.532	0.978
80222	Boston Area	2	1	13-13	27.960	30.693	29.980	0.911	0.933
80222	Boston Area	2	1	14-14	20.990	29.349	29.140	0.715	0.720
80222	Boston Area	2	1	15-15	31.060	21.793	21.870	1.425	1.420
80222	Boston Area	2	1	16-16	43.910	29.423	27.330	1.492	1.607
80222	Boston Area	2	1	16-16	32.980	28.095	27.870	1.174	1.183
80222	Boston Area	2	1	17-17	30.020	47.401	48.540	0.633	0.618
AVERAGES:					62.436	65.260	63.792	1.104	1.116

TABLE 8.6. SUMMARY OF NMHC CONCENTRATIONS, OBSERVED AND PREDICTED, ALOFT OVER THE NON-URBAN AREAS DURING THE 1980 SUMMER PERIOD.

DATE	LOCATION	ROW LAYERS	N TIME PERIOD (hr, LST)	NMHC(O) (ppbC)	NMHC(PT) (ppbC)	NMHC(P2) (ppbC)	O/PT RATIO	O/P2 RATIO
New York-Vermont area:								
80218	N.Y.-Vermont	2	1 17-17	26.400	26.738	26.190	0.987	1.008
80220	Finger Lakes Area	2	1 16-16	31.290	22.535	22.590	1.389	1.385
80221	Fing. Lakes-N.Y.	1	1 8- 8	87.500	37.557	39.260	2.330	2.229
80221	Hudson Valley	1	2 12-12	23.955	21.743	23.565	1.102	1.017
80221	Vermont	1	1 15-15	24.820	25.229	24.300	0.984	1.021
AVERAGES:				38.793	26.760	27.181	1.358	1.332
Pennsylvania-Maryland area:								
80209	North. Maryland	2	4 12-13	33.793	30.940	31.285	1.092	1.080
80209	So. Cen. Penn.	1 2	4 17-19	20.175	45.934	41.963	0.439	0.481
80213	W.VA.-Penn. Area	2	1 7- 7	53.510	24.004	25.890	2.229	2.067
80213	Central Penn.	2	1 17-17	25.200	18.764	23.030	1.343	1.094
80213	NW Penn. Area	2	1 18-18	92.370	30.440	34.870	3.035	2.649
80213	Central Penn.	2	1 18-18	36.600	29.995	30.800	1.220	1.188
80213	Central Penn.	2	1 19-19	41.210	29.241	30.040	1.409	1.372
80213	North. Maryland	2	1 20-20	35.610	40.336	42.290	0.883	0.842
80219	Penn. Area	2	1 1- 1	18.890	20.150	19.020	0.937	0.993
80219	W.VA.-Penn. Area	2	1 2- 2	27.600	20.190	21.670	1.367	1.274
80220	Penn. Area	2	1 22-22	23.740	20.917	22.940	1.135	1.035
80220	Penn. Area	2	1 22-22	20.470	22.052	21.880	0.928	0.936
80221	Delaware Valley	2	1 14-14	41.060	28.916	26.650	1.420	1.541
80227	N. Philadelphia	1 2	3 15-16	65.477	26.580	45.463	2.463	1.440
AVERAGES:				38.265	27.747	29.842	1.421	1.285
Eastern Ohio area:								
80206	Eastern Ohio	2	2 9- 9	138.125	17.850	15.040	7.738	9.184
80206	Ohio Area	2	2 17-18	49.505	13.965	14.970	3.545	3.307
80206	Ohio Area	1 2	2 20-20	52.205	23.607	20.910	2.211	2.497
80207	Ohio Area	2	4 12-13	60.270	41.544	34.035	1.451	1.771
80207	Columbus, Ohio	2	2 16-17	51.200	19.644	22.935	2.606	2.232
80208	Columbus, Ohio	1	1 8- 8	112.540	29.798	25.440	3.777	4.424
80208	Eastern Ohio	2	2 10-10	48.570	13.641	14.100	3.561	3.445
80208	Eastern Ohio	2	1 12-12	35.600	10.543	10.730	3.377	3.318
80208	Columbus, Ohio	2	2 16-16	80.765	21.759	15.805	3.712	5.110
80211	Columbus, Ohio	2	2 19-20	33.550	34.037	26.400	0.986	1.271
80212	Columbus, Ohio	2	1 7- 7	29.820	34.621	29.730	0.861	1.003
80212	Columbus, Ohio	3	1 8- 8	28.150	20.205	13.570	1.393	2.074
80212	Columbus, Ohio	2	4 10-11	65.235	28.437	21.833	2.294	2.988
80212	Ohio Area	2	3 12-14	98.413	25.081	22.367	3.924	4.400
80212	Columbus, Ohio	1	1 20-20	30.090	157.377	90.920	0.191	0.331
80212	Ohio-W.Va.	2	2 21-22	56.295	14.002	13.960	4.020	4.033
80213	Columbus, Ohio	1	2 12-12	65.415	28.593	23.290	2.288	2.809
80213	Columbus, Ohio	1 2	4 12-15	56.300	25.055	25.398	2.247	2.217
80213	Columbus, Ohio	2	2 19-19	72.605	18.896	18.665	3.842	3.890
80213	Columbus, Ohio	1	1 20-20	162.500	62.496	63.930	2.600	2.542
80214	Ohio Area	2	1 15-15	54.570	13.505	13.930	4.041	3.917
80214	Ohio Area	2	1 19-19	41.560	19.570	19.470	2.124	2.135
80214	Ohio Area	2	1 20-20	50.270	22.063	23.190	2.278	2.168
80215	Central Ohio	1 2	2 14-14	43.015	14.873	17.325	2.892	2.483
80215	Columbus, Ohio	3	1 14-14	23.810	3.207	3.450	7.425	6.901
80217	Columbus, Ohio	1 2	2 5- 6	36.715	22.908	30.960	1.603	1.186
80217	Columbus, Ohio	2	1 11-11	43.100	28.110	26.260	1.533	1.641
80217	Columbus, Ohio	2	3 12-14	61.470	30.638	21.447	2.006	2.866
80217	Columbus, Ohio	1 2	3 14-15	57.827	16.953	14.707	3.411	3.932
80217	Ohio Area	1	1 14-14	46.230	17.983	17.720	2.571	2.609
80217	Columbus, Ohio	2	3 20-21	48.823	7.717	7.720	6.327	6.324
80219	Ohio-Kentucky	2	1 13-13	16.970	18.037	15.600	0.941	1.088
80220	NE Ohio Area	1	1 19-19	27.340	43.856	44.410	0.623	0.616
AVERAGES:				56.935	27.290	23.643	2.861	3.052

over the urban areas. There were also fewer samples used in the rural analyses than in the urban. For eastern OH, which has a mix of rural and semi-urban aircraft samples, the average observed NMHC value was 57 ppbC compared to 27 ppbC predicted, an underprediction of 53%. While the eastern OH predicted values appeared more like the other predicted rural values, the observed concentrations in eastern OH showed some higher values, definitely showing source influences. In the Columbus area the ROM predicted NMHC values of the same magnitude as the observations, but not necessarily on the same day, for high concentration events. See, for example, day 80212 where the observed and predicted values were 30 and 157 ppbC, respectively, and day 80213 where the observed and predicted values were 162 and 62 ppbC, respectively. This may have had to do with plume misalignment.

These data are also shown in scatterplot form in Figures 8.95 and 8.96. Figure 8.95 presents the comparison of predicted vs. observed NMHC data for the urban areas, and Figure 8.96 presents the comparison for non-urban areas. The straight line in the figures is the line of perfect agreement. Although there is considerable scatter among the points for a given city area, a clear trend emerges. For Baltimore, Boston, and New York, the data are scattered about the line of perfect agreement. The average O/P ratios for these cities lie between 1 and 2. The data for Washington are nearly all underpredicted, and the tabular ratio for Washington shows a value of 2.8. Several of the cities, especially for Baltimore, show a significant number of outlier data points, all on the underpredictive side. There are generally fewer data points on the non-urban scatterplots than on the urban ones. The data are more consistently underpredicted on the non-urban plots and are generally at lower observed NMHC concentrations. For the PA-MD and NY-VT plots, if the few most extreme underpredictive outliers were eliminated, the results would show nearly perfect agreement between observations and predictions.

As in the surface NMHC analysis, we have selected several samples from the aloft data base for reactivity analysis. Three NMHC data values from each of the urban analyses, and two each from the non-urban analyses, were selected as representative of the entire sample. The PA-MD and NY-VT non-urban samples were combined here as the NY-PA data set. The data points selected are shown in tabular form in Appendix J. Since each data point in our data base can contain more than one NMHC sample, averaged over space and time, there are actually more than 2 or 3 samples included in the reactivity analysis for each geographic area. As discussed previously, the oxygenated component of the observed data is essentially unmeasured by the chromatographic analysis. Therefore, we have added sufficient oxygenated hydrocarbons to the observed NMHC concentration such that the carbon-percent of oxygenates in the observations was equal to the carbon-percent of oxygenates in the predictions. This mass was added only for the reactivity analysis; it was not considered in the previous total NMHC comparisons.

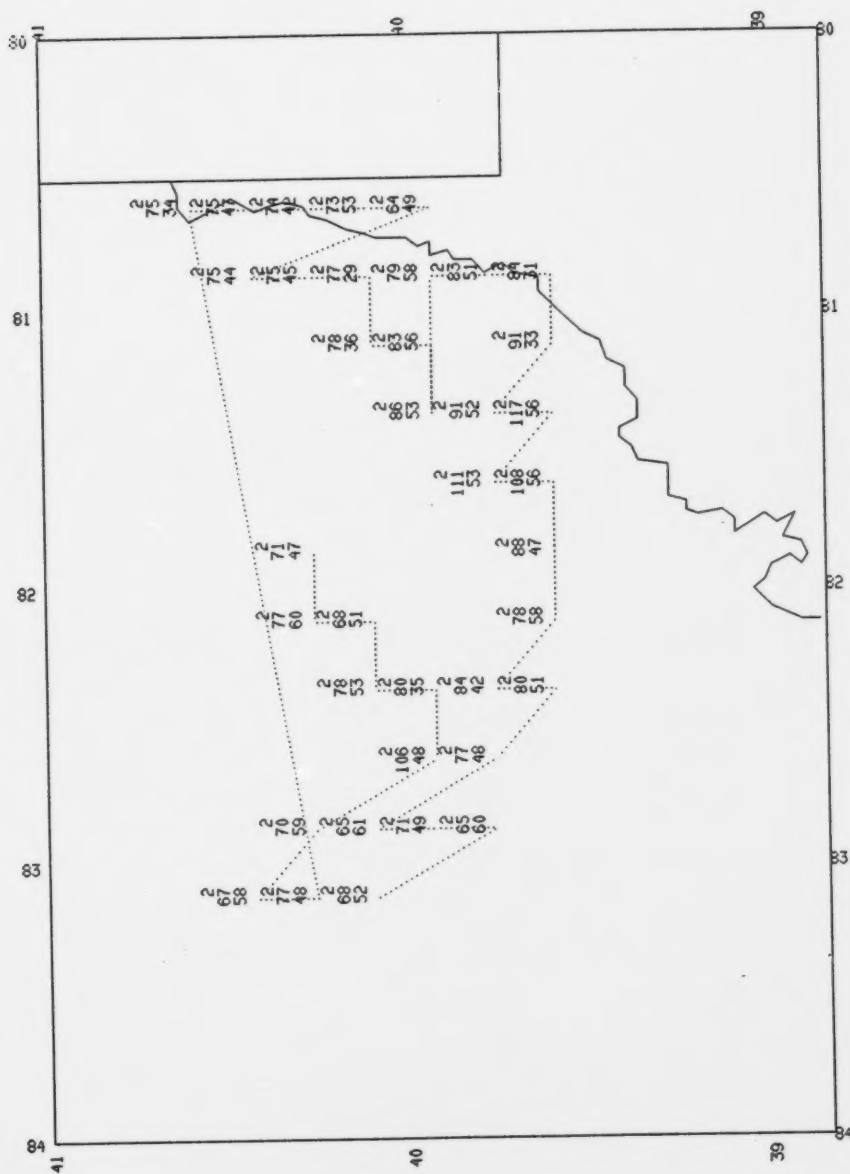
The results of the reactivity analysis are shown in Table 8.7. The NMHC

TABLE 8.7. SUMMARY OF SELECTED REACTIVITY CLASS PROFILES OF NMHC CONCENTRATIONS ALOFT

Area	NMHC (ppbC)	%ETH	%OLE	%PAR	%TOL	%XYL	%ISOP	%NONR	%OXY
	Observed —>	Predicted —>							
	Obs./Pred. —>								
Boston	105.85	6.95	0.44	52.96	9.63	6.76	0.00	11.95	11.35
	86.45	3.09	1.08	73.43	5.23	1.43	0.09	4.31	11.35
	1.22	2.25	0.41	0.72	1.84	4.72	0.00	2.77	1.00
New York	123.35	2.51	0.49	54.43	12.19	11.04	0.75	9.84	8.98
	108.60	2.06	1.52	75.20	4.88	1.52	0.65	5.19	8.98
	1.14	1.22	0.32	0.72	2.50	7.26	1.15	1.90	1.00
Baltimore	120.39	3.17	0.76	49.77	9.08	11.36	0.00	14.97	10.87
	74.92	2.18	0.80	74.30	4.32	0.75	0.15	6.64	10.87
	1.61	1.46	0.95	0.67	2.10	15.08	0.00	2.26	1.00
Washington	275.89	9.59	0.56	52.06	8.29	10.51	0.00	7.89	11.09
	106.28	4.32	4.07	65.79	6.64	3.13	0.29	4.67	11.09
	2.60	2.22	0.14	0.79	1.25	3.36	0.00	1.69	1.00
Ohio	62.17	2.38	0.65	55.45	3.79	5.31	0.34	19.00	11.99
	31.80	2.20	1.25	74.43	3.74	0.74	0.52	5.14	11.99
	1.96	1.05	0.52	0.74	1.01	7.18	0.65	3.70	1.00
NY-PA	30.65	1.69	0.00	39.49	2.37	7.28	0.00	33.74	15.45
	21.73	3.72	2.12	71.94	1.70	0.49	1.58	3.00	15.45
	1.41	0.45	0.00	0.55	1.40	14.85	0.00	11.26	1.00

concentrations and the carbon-percent of each reactivity component for the samples selected from each geographic area were averaged to produce the results shown in the table. Average observed and predicted NMHC concentrations are shown, as are the averaged observed and predicted carbon-percents from the reactivity components. The oxygenated component is the same in observed and predicted data because we have added compensating mass to the observed data to assure a match for this category. The results show general overprediction of the carbon-percents for the olefin, paraffin, and isoprene categories. The greatest underpredictions occurred in the categories of non-reactives and xylene with ethylene and toluene showing smaller values of underprediction. The carbon-percents of the various categories were similar for the aloft data compared to the surface data, although NMHC concentrations were much lower aloft.

It is interesting to note that the categories of underpredicted NMHC aloft are also those categories containing biogenic NMHC emissions. There may be some indication here that the amount of biogenic organics in the emissions inventory is overestimated. Added evidence for this point is seen in the opposite indications for ethylene and olefins, both of which have a strong mobile-source emissions component. If the effect were primarily from anthropogenic sources, both ethylene and olefins should be over- or underpredicted together. The fact that they show different behavior indicates that there is another factor, most likely biogenic organics lumped as olefins, that have caused the overprediction of olefins. Another possible explanation for this occurrence is that the influence of the biogenic species is most pronounced near the surface since the biogenic emissions are entirely from area sources and are generally fast-reacting species. With increasing altitude above the surface we would expect to find less of the biogenic material. The ROM's two-layer structure within the boundary layer may not afford the vertical resolution necessary to define the vertical gradient in primary biogenic VOCs. The fact that the predicted and observed surface isoprene concentrations were in fairly good agreement lends some support to this argument. There is, yet, considerable uncertainty concerning the magnitude and distribution of biogenic emissions. Much more research needs to be accomplished in this area before the true influence of these emissions is known on the regional O₃ problem.



COLUMBUS-H.VA. (REGIONAL) 7/30/80 (HRS 20-22)

WINDOW extent - rows 6:18 cols 1:16

Figure 8.1. Geographical distribution of selected O₃ data from flight on July 30, 1980 from OH to WV. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - COLUMBUS-W.VA. (PLUME)
JULY 30, 1980 (AV)
LAYER 2

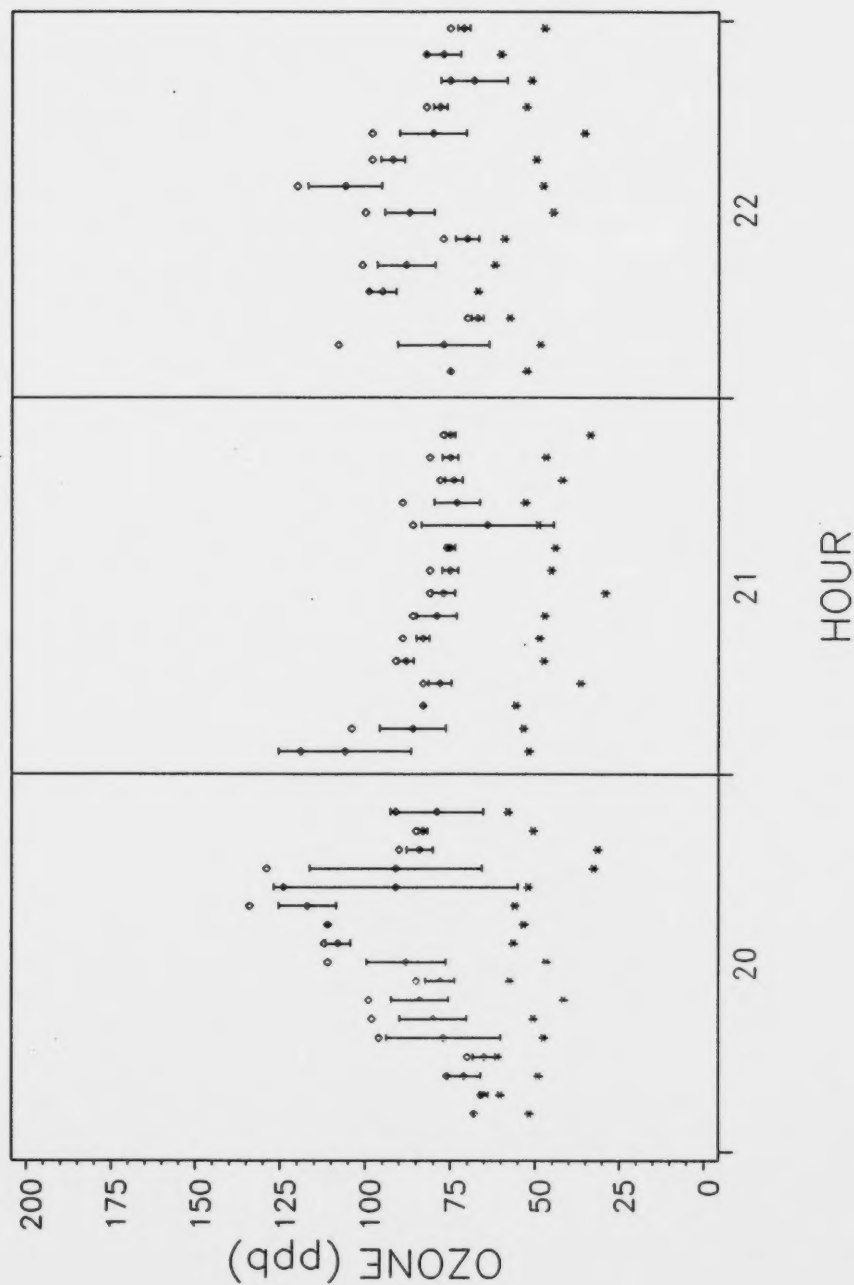


Figure 8.2. Time series of O_3 data from flight on July 30, 1980 from OH to WV. Within each hour period, for each ROM grid cell traversed by the aircraft, the observed mean concentration (diamond) is surrounded by the observed standard deviation with the observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

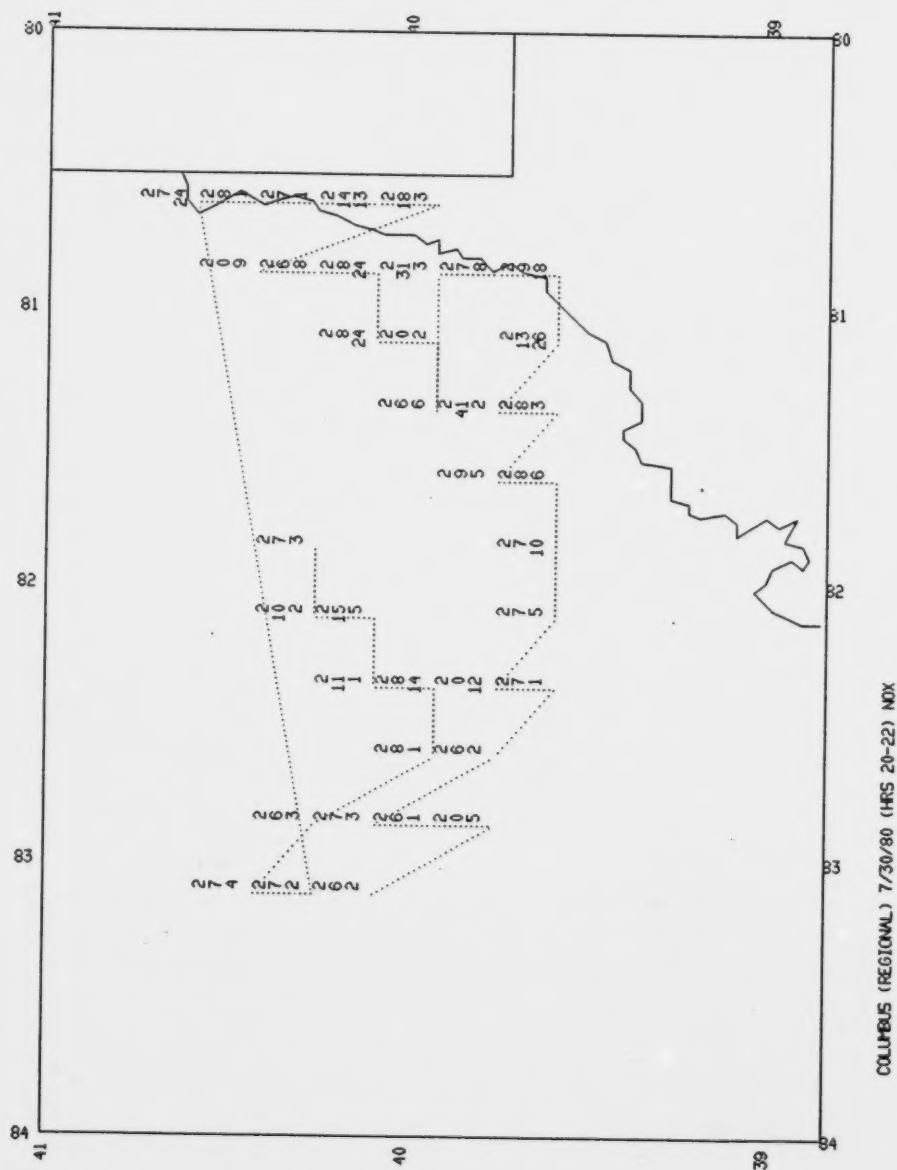


Figure 8.3. Geographical distribution of selected NO_x data from flight on July 30, 1980 from OH to WV. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - COLUMBUS-W.VA. (PLUME)
JULY 30, 1980 (AV)
LAYER 2

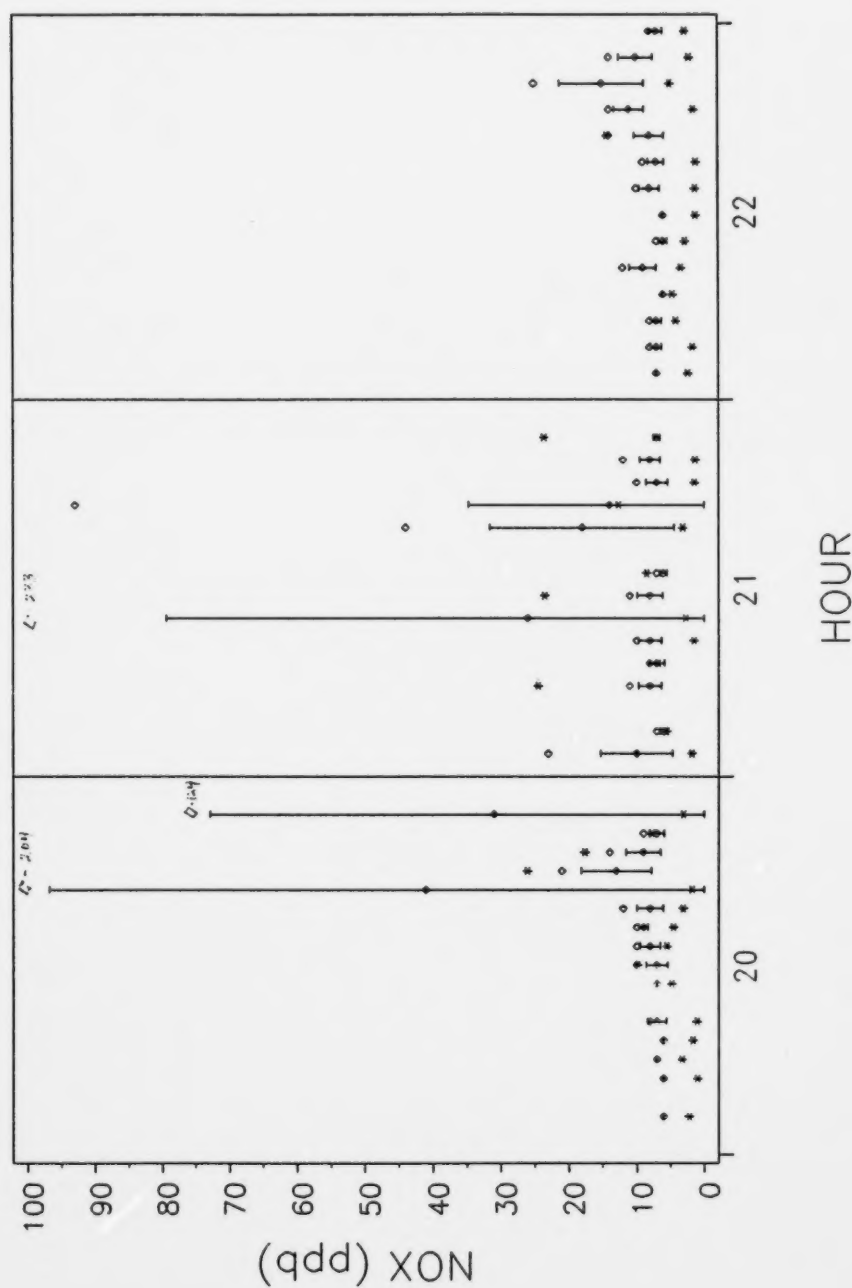


Figure 8.4. Time series of NO_x data from flight on July 30, 1980 from OH to WV. Within each hour period, for each ROM grid cell traversed by the aircraft, the observed mean concentration (diamond) is surrounded by the observed standard deviation with the observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

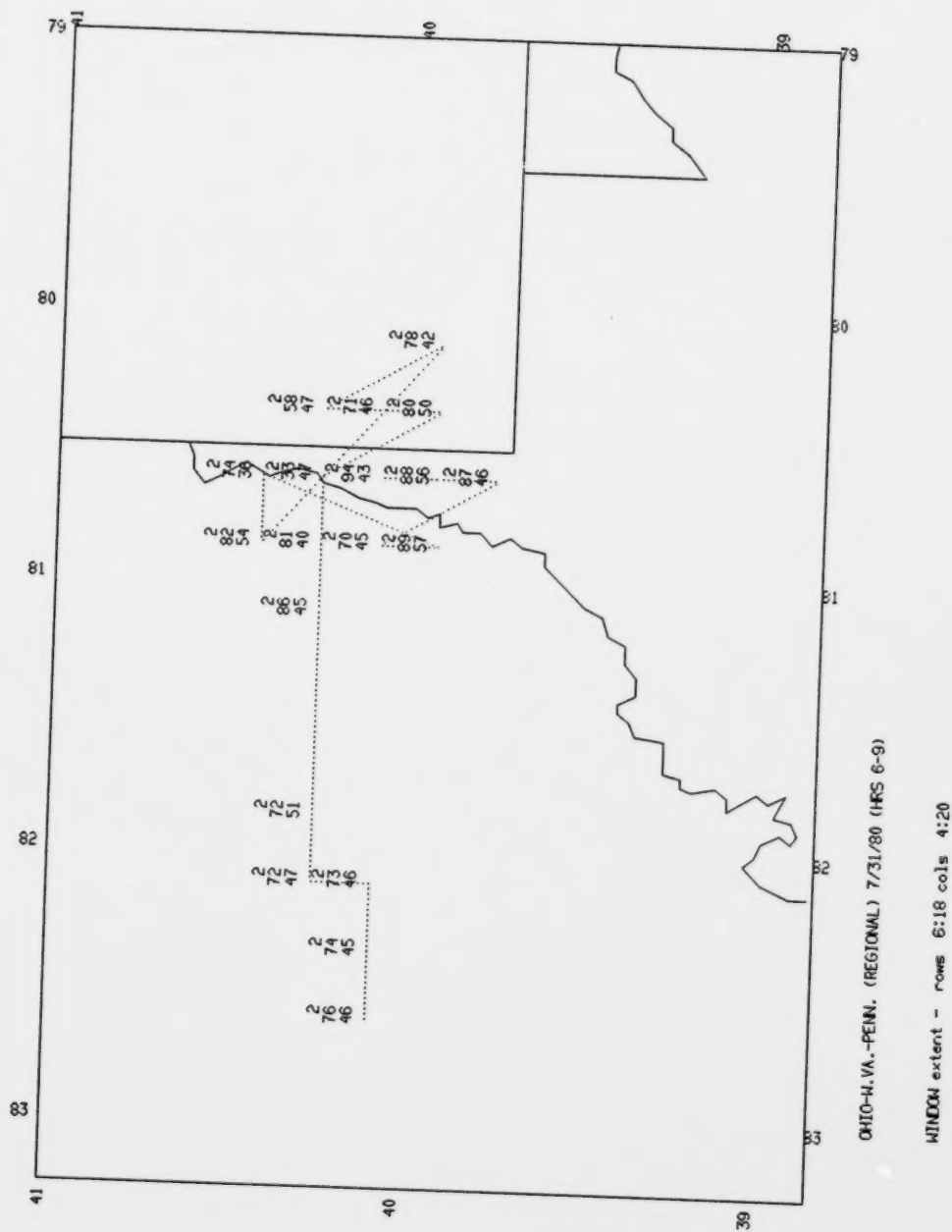


Figure 8.5. Geographical distribution of selected O₃ data from flight on July 31, 1980 from Columbus, OH to Pittsburgh, PA. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - OHIO-W.VA.-PA. (REGIONAL)
JULY 31, 1980 (SRI)
LAYER 2

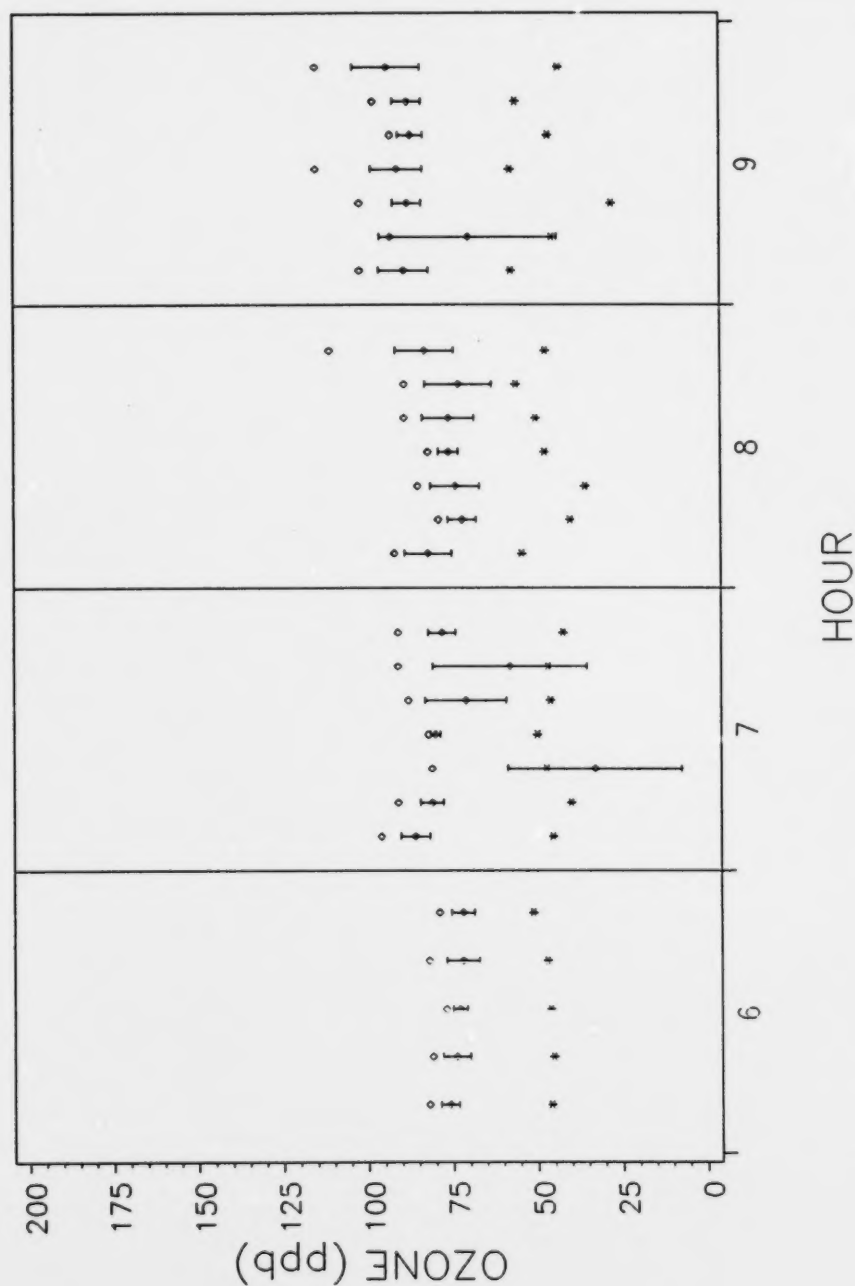


Figure 8.6. Time series of O_3 data from flight on July 31, 1980 from Columbus, OH to Pittsburgh, PA. Within each hour period, for each ROM grid cell traversed by the aircraft, the observed mean concentration (diamond) is surrounded by the observed standard deviation with the observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

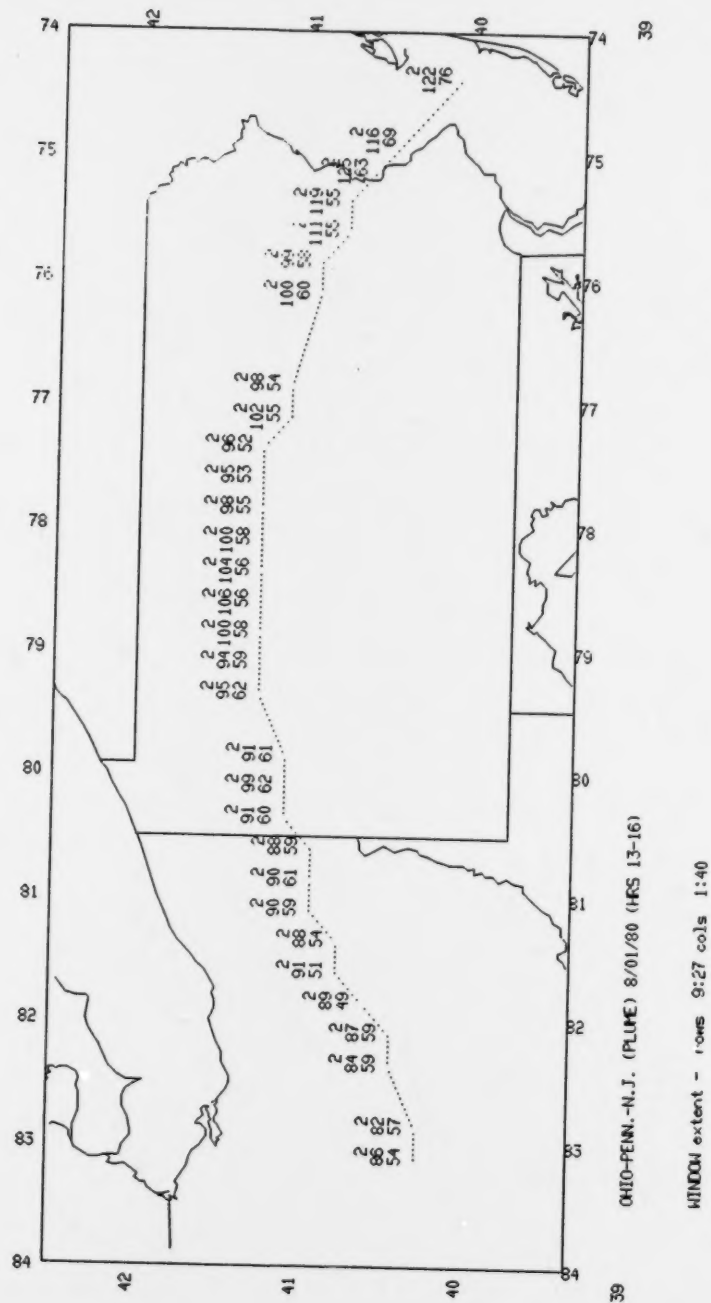


Figure 8.7. Geographical distribution of selected O₃ data from flight on Aug. 1, 1980 from OH to NJ. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - OHIO-PA.-N.J. (PLUME)
AUGUST 1, 1980 (AV)
LAYER 2

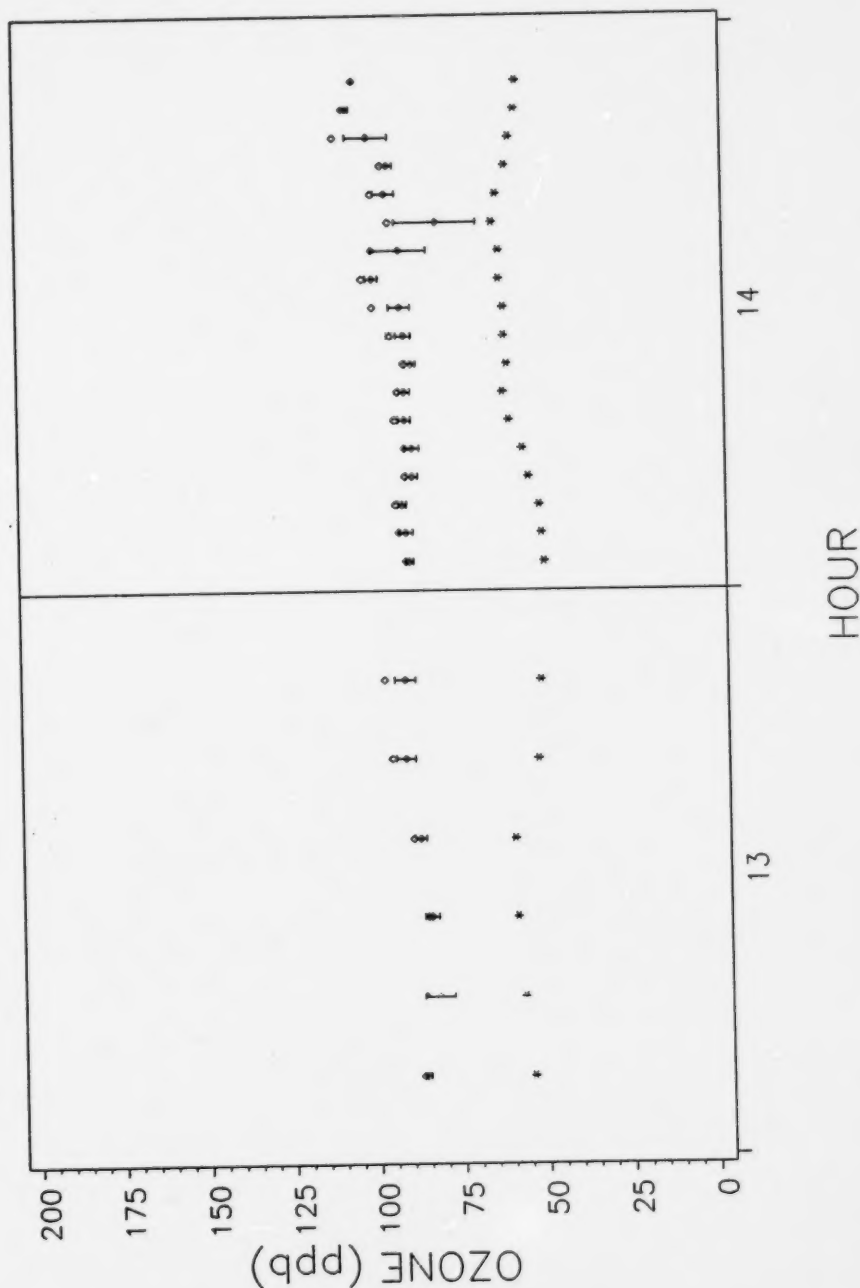


Figure 8.8. Time series of O₃ data from flight on Aug. 1, 1980 from OH to NJ. Within each hour period, for each ROM grid cell traversed by the aircraft, the observed mean concentration (diamond) is surrounded by the observed standard deviation with the observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

AIRCRAFT - OHIO-PA.-N.J. (PLUME)
 AUGUST 1, 1980 (AV)
 LAYER 2

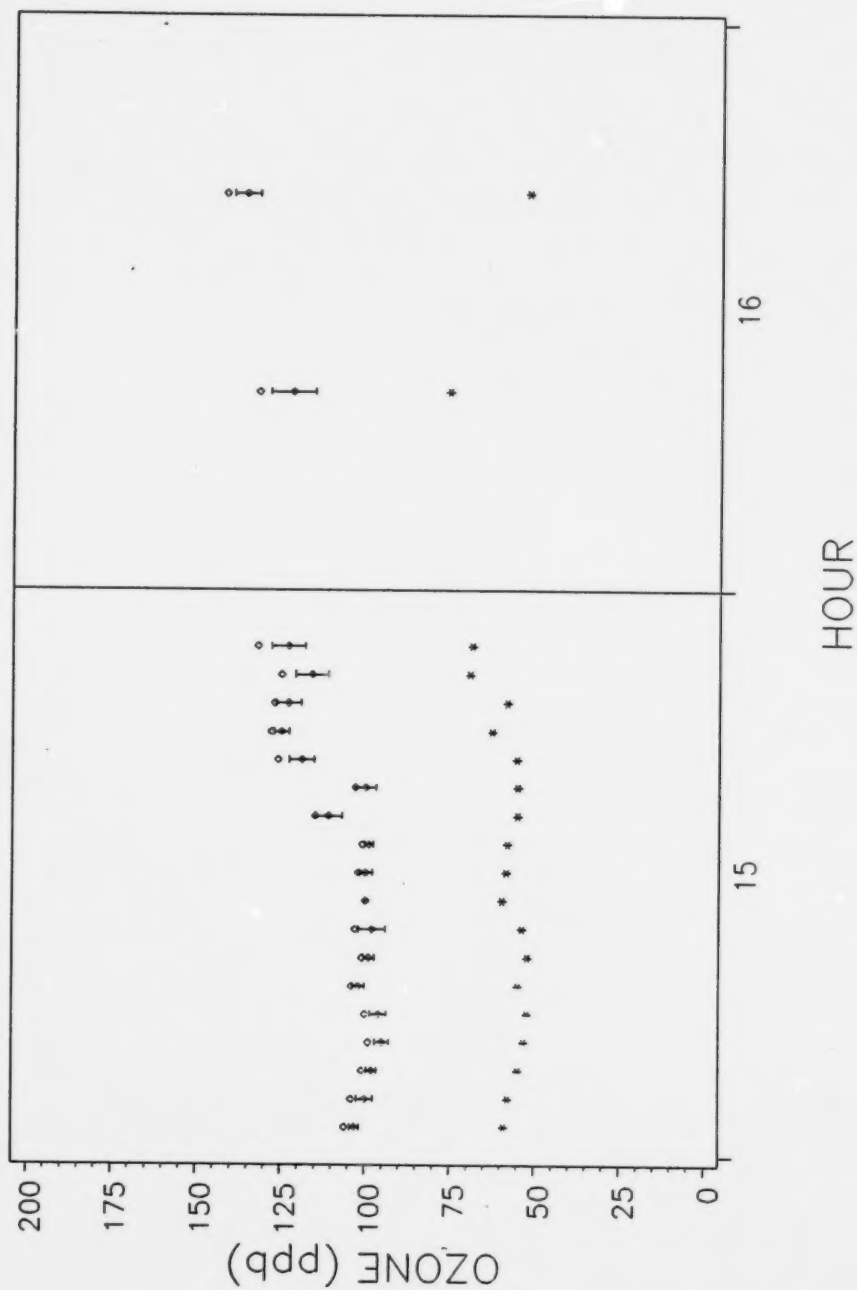


Figure 8.8 (cont.)

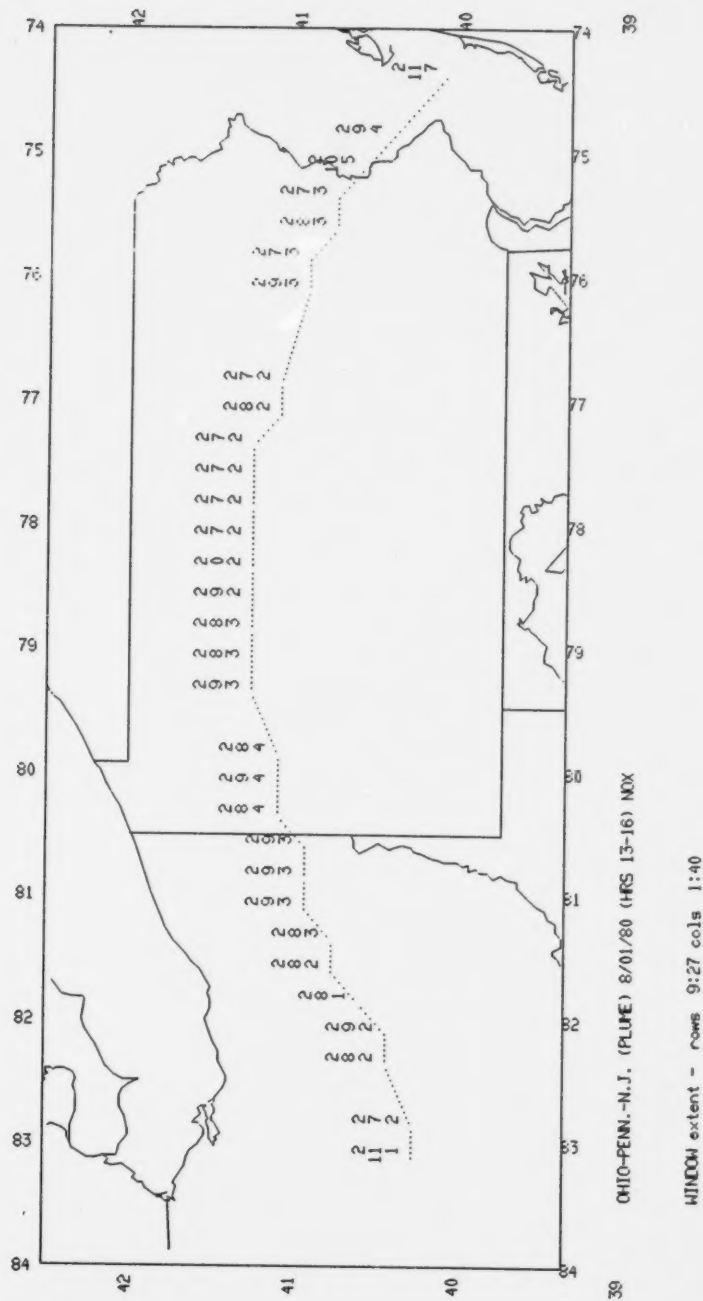


Figure 8.9. Geographical distribution of selected NO_x data from flight on Aug. 1, 1980 from OH to NJ. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - OHIO-PA.-N.J. (PLUME)
 AUGUST 1, 1980 (AV)
 LAYER 2

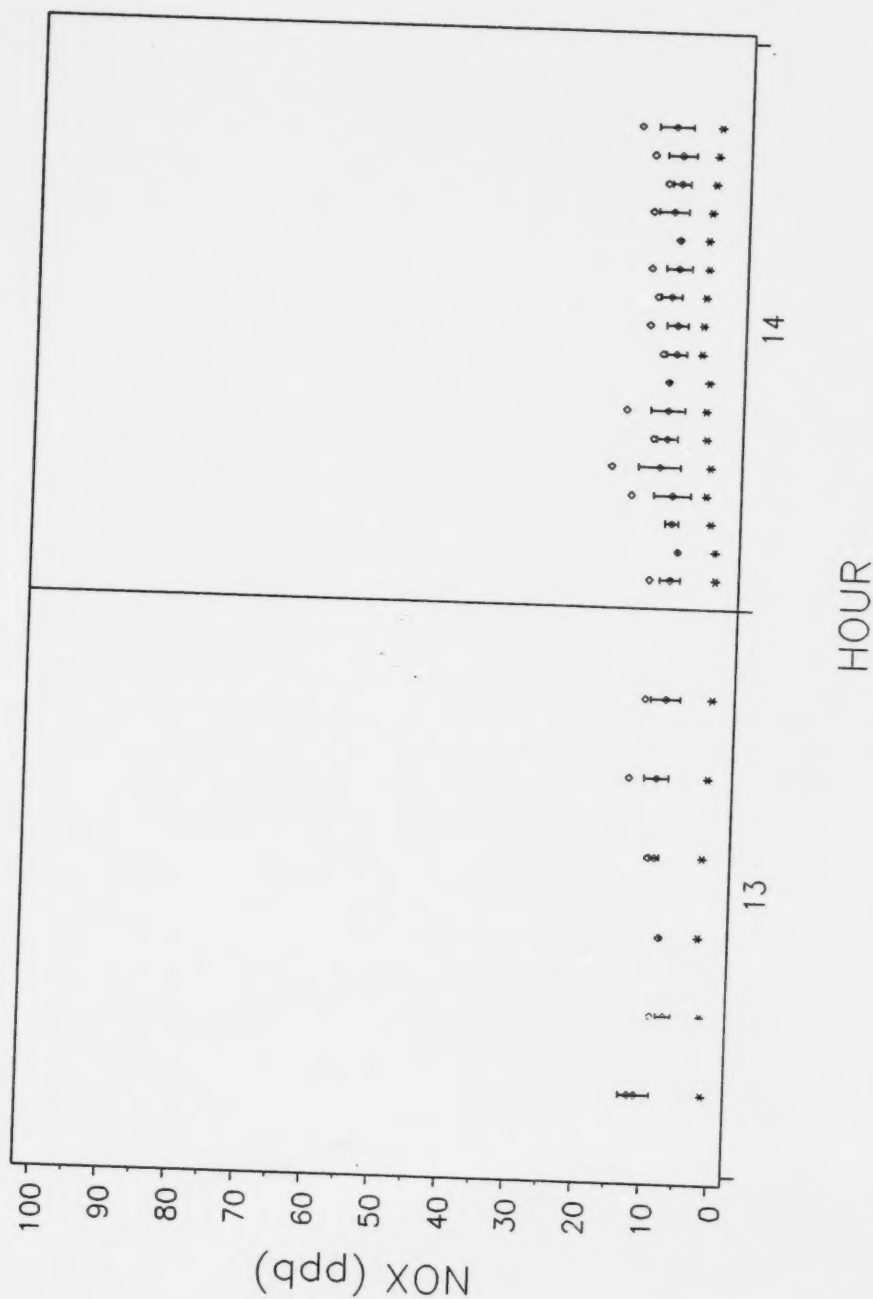


Figure 8.10. Time series of NO_x data from flight on Aug. 1, 1980 from OH to NJ. Within each hour period, for each ROM grid cell traversed by the aircraft, the observed mean concentration (diamond) is surrounded by the observed standard deviation with the observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

AIRCRAFT - OHIO-PA.-N.J. (PLUME)
 AUGUST 1, 1980 (AV)
 LAYER 2

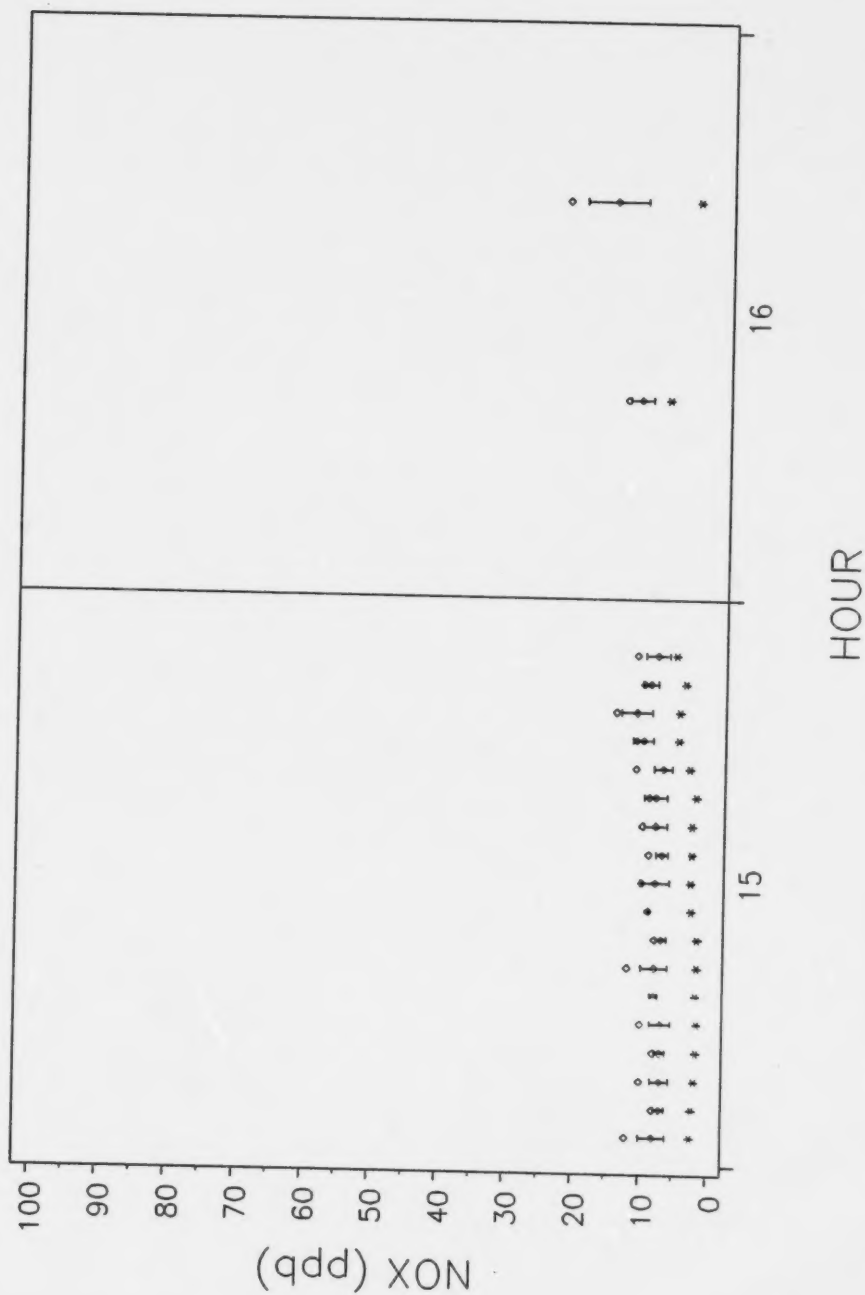


Figure 8.10 (cont..)

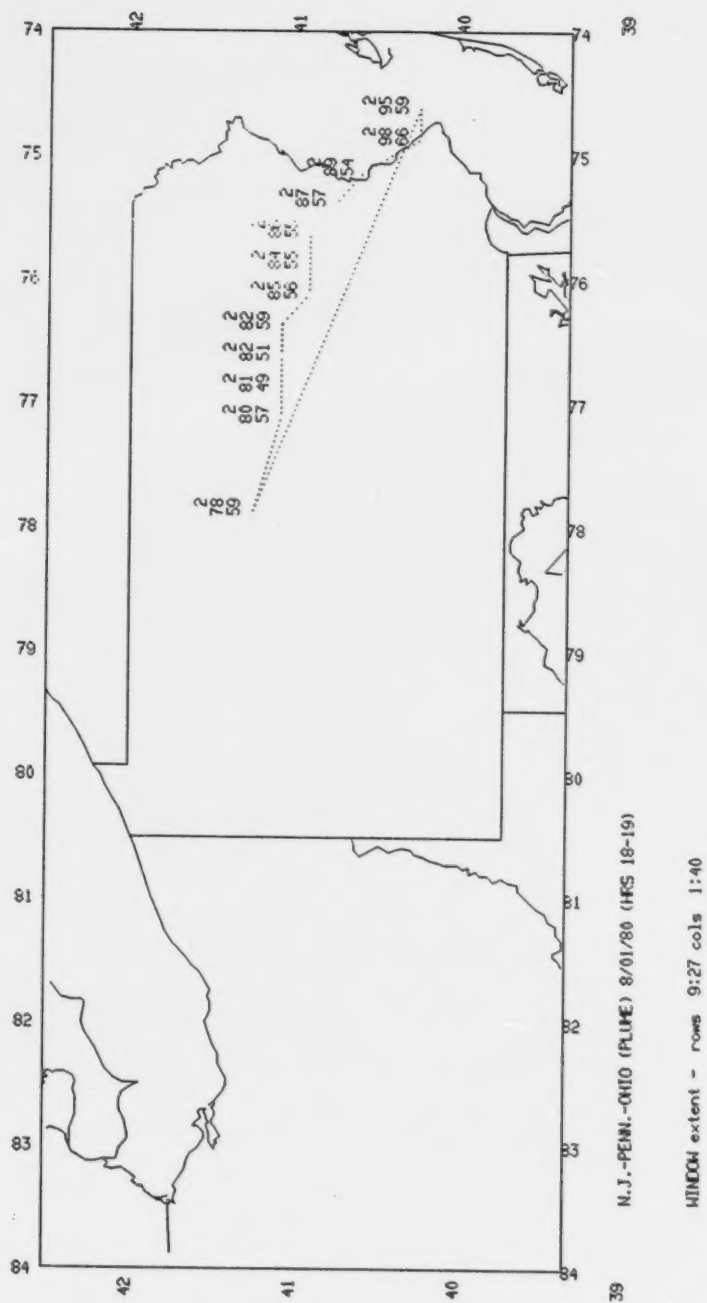


Figure 8.11. Geographical distribution of selected O_3 data from flight on Aug. 1, 1980 from NJ to PA. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - N.J.-PA.-OHIO (PLUME)
AUGUST 1, 1980 (AV)
LAYER 2

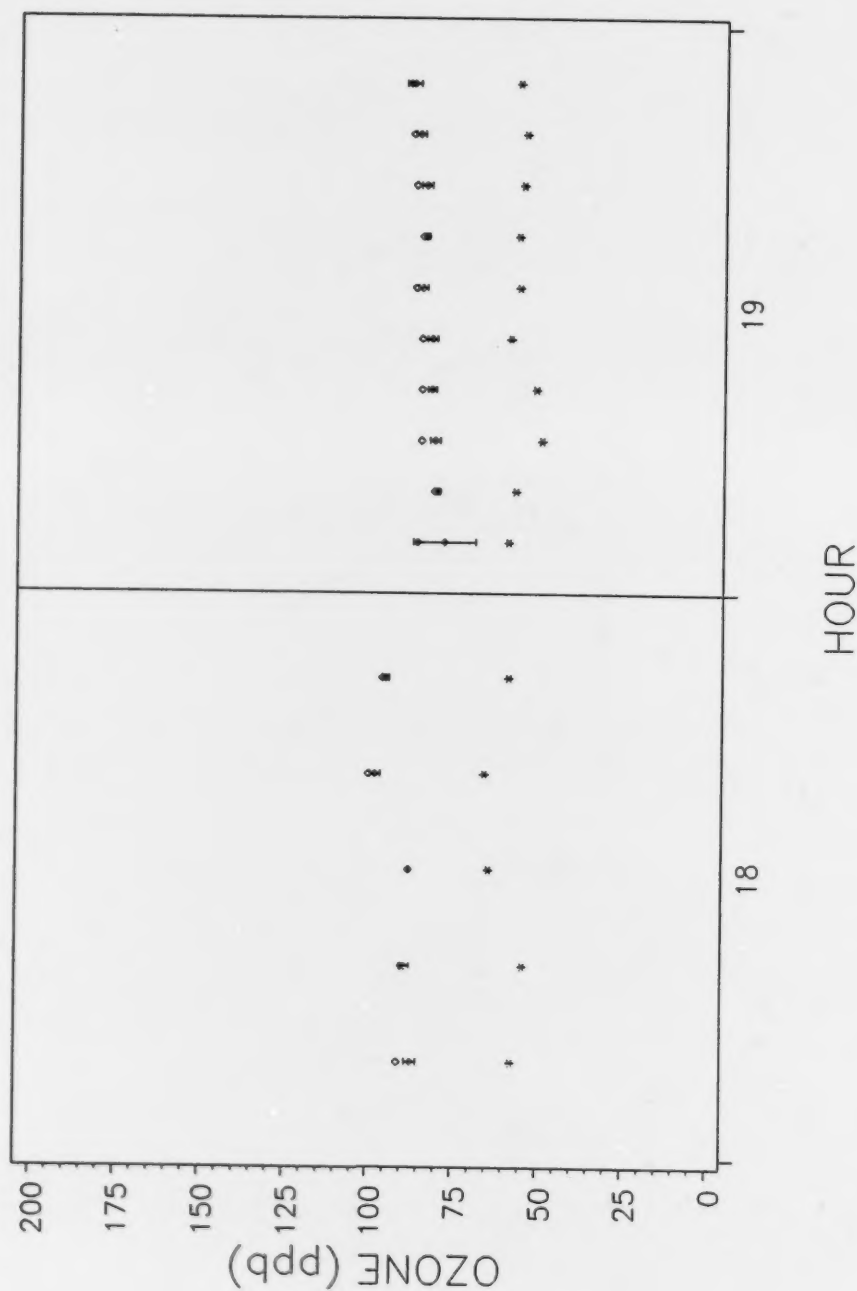


Figure 8.12. Time series of O_3 data from flight on Aug. 1, 1980 from NJ to PA. Within each hour period, for each ROM grid cell traversed by the aircraft, the observed mean concentration (diamond) is surrounded by the observed standard deviation with the observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

AIRCRAFT - N.J.-PA.-OHIO (PLUME)
AUGUST 1, 1980 (AV)
LAYER 2

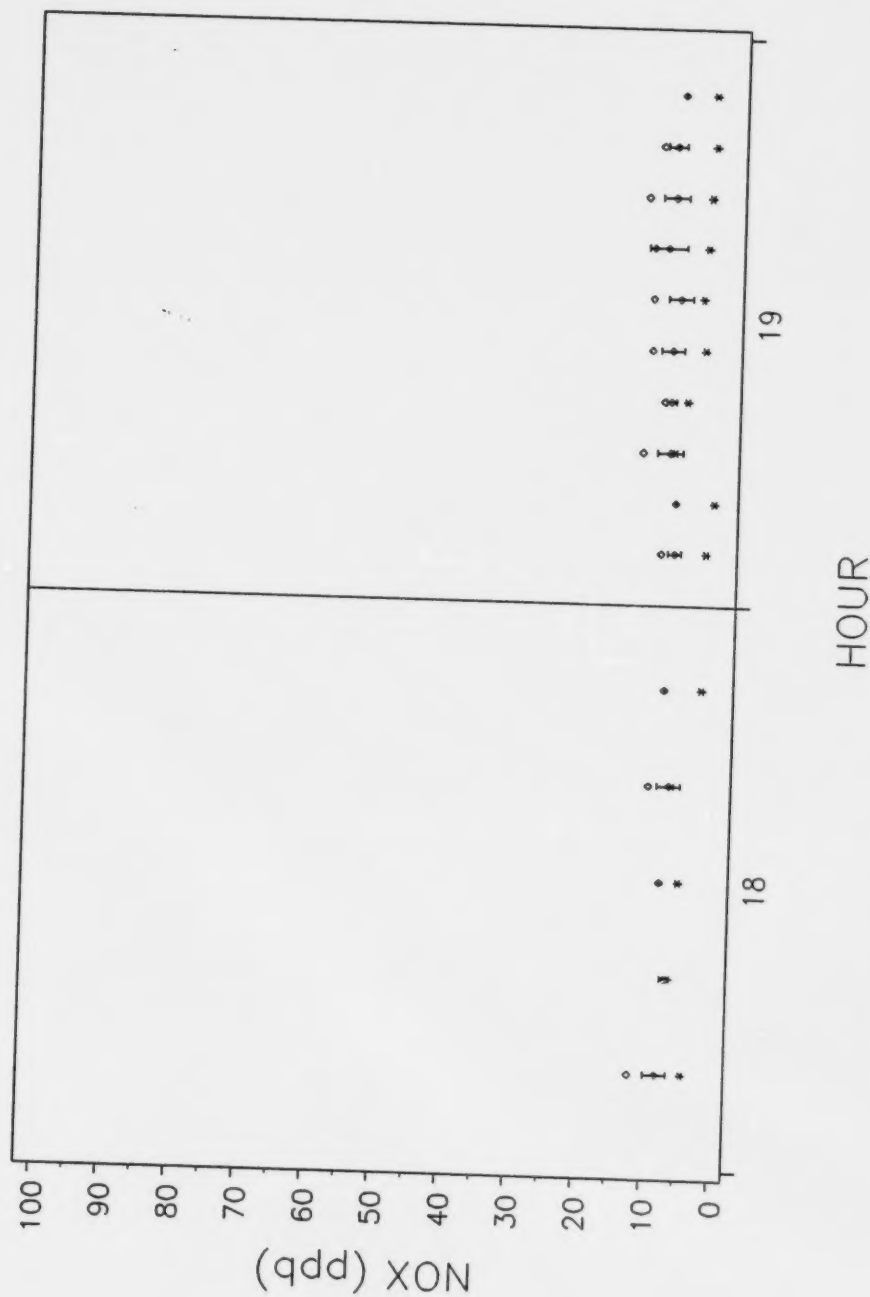


Figure 8.14. Time series of NO_x data from flight on Aug. 1, 1980 from NJ to PA. Within each hour period, for each ROM grid cell traversed by the aircraft, the observed mean concentration (diamond) is surrounded by the observed standard deviation with the observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

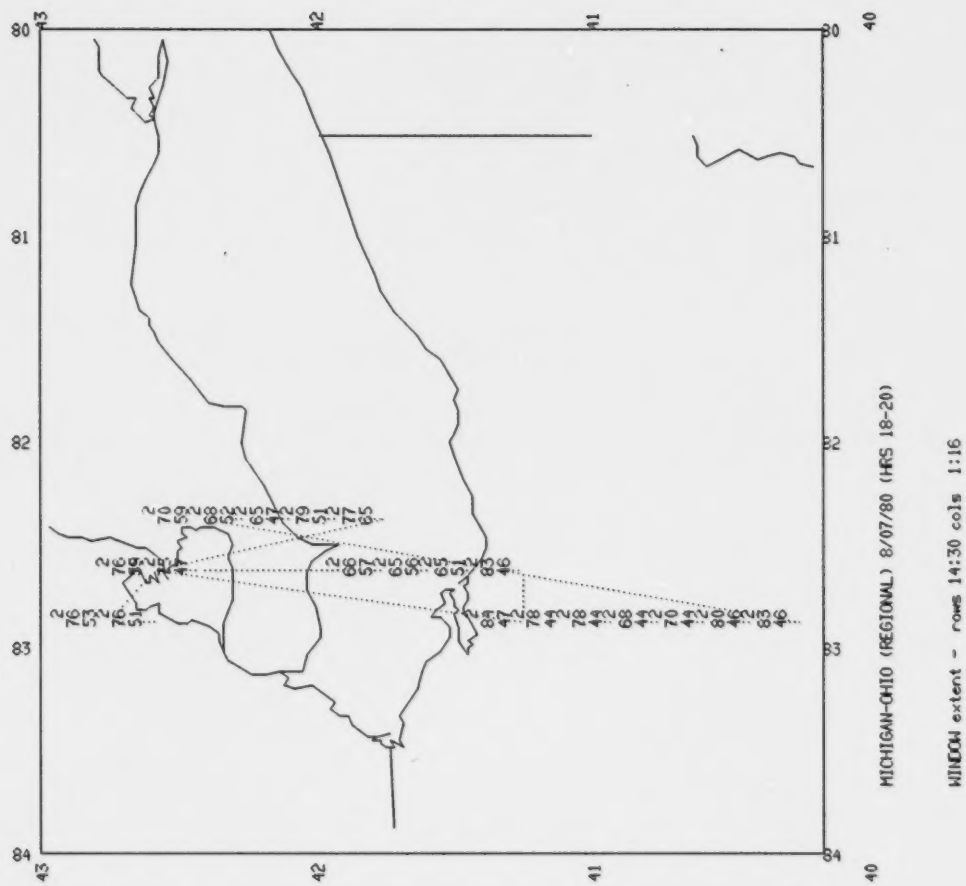


Figure 8.15. Geographical distribution of selected O_3 data from flight on Aug. 7, 1980 from MI to OH. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - MI.-OHIO (REGIONAL)
AUGUST 7, 1980 (SRI)
LAYER 2

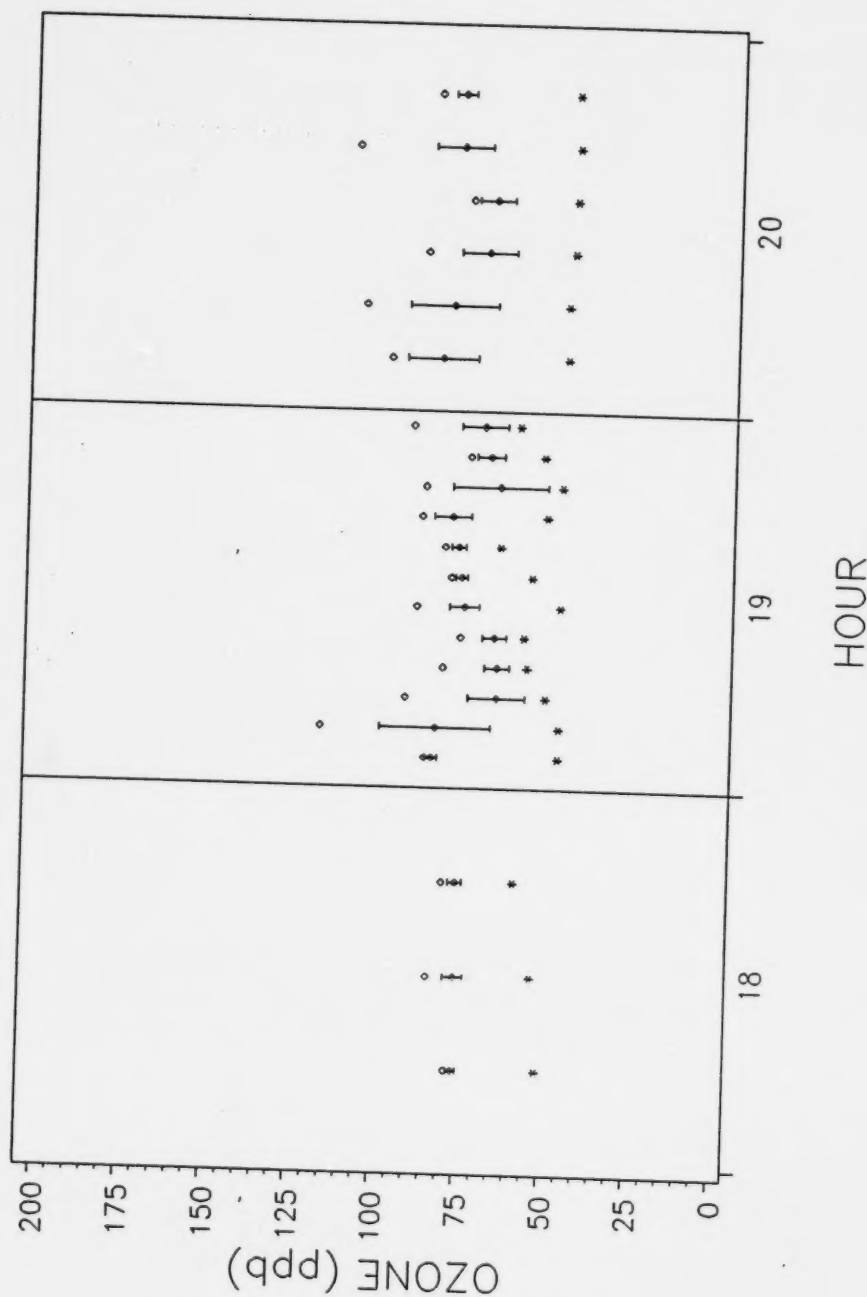


Figure 8.16. Time series of O_3 data from flight on Aug. 7, 1980 from MI to OH. Within each hour period, for each ROM grid cell traversed by the aircraft, the observed mean concentration (diamond) is surrounded by the observed standard deviation with the observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

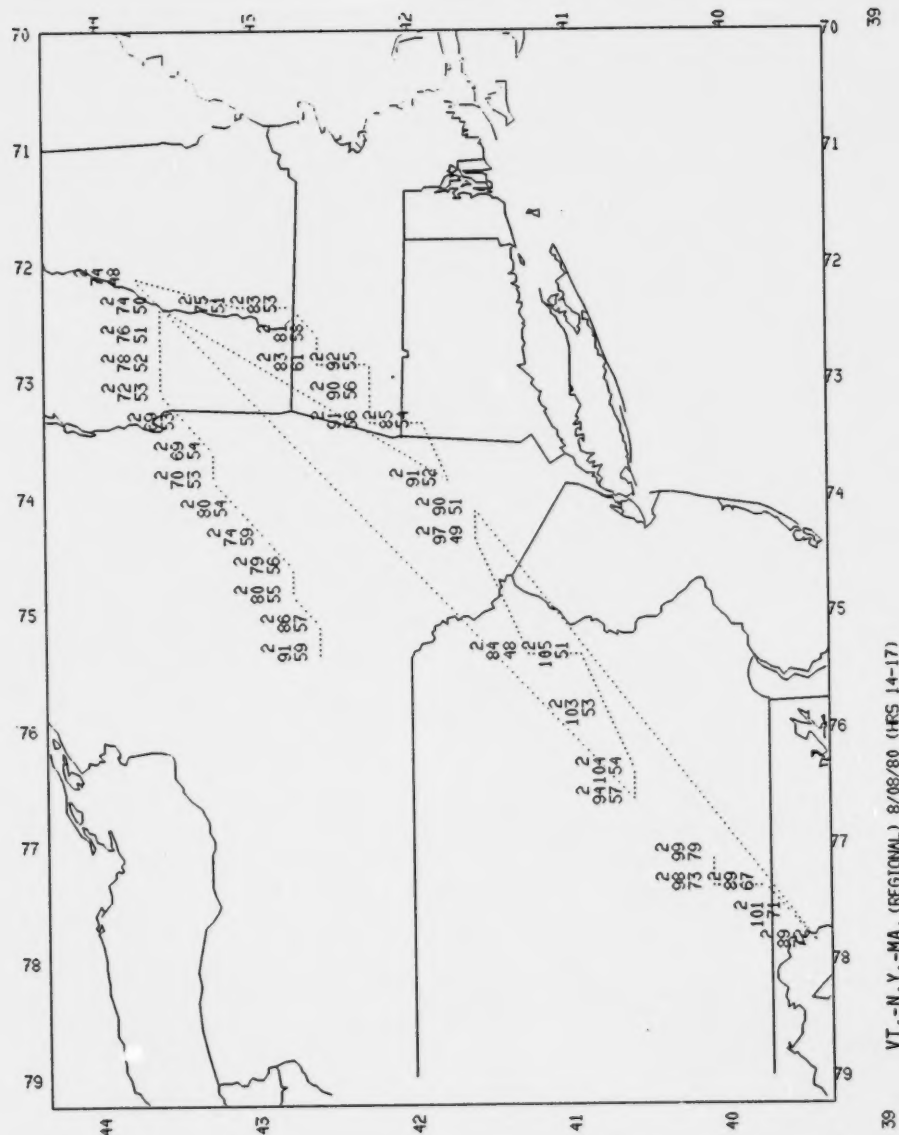


Figure 8.17. Geographical distribution of selected O₃ data from flight on Aug. 8, 1980 from VT to PA. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - VT.-N.Y.-MA. (REGIONAL)
 AUGUST 8, 1980 (AV)
 LAYER 2

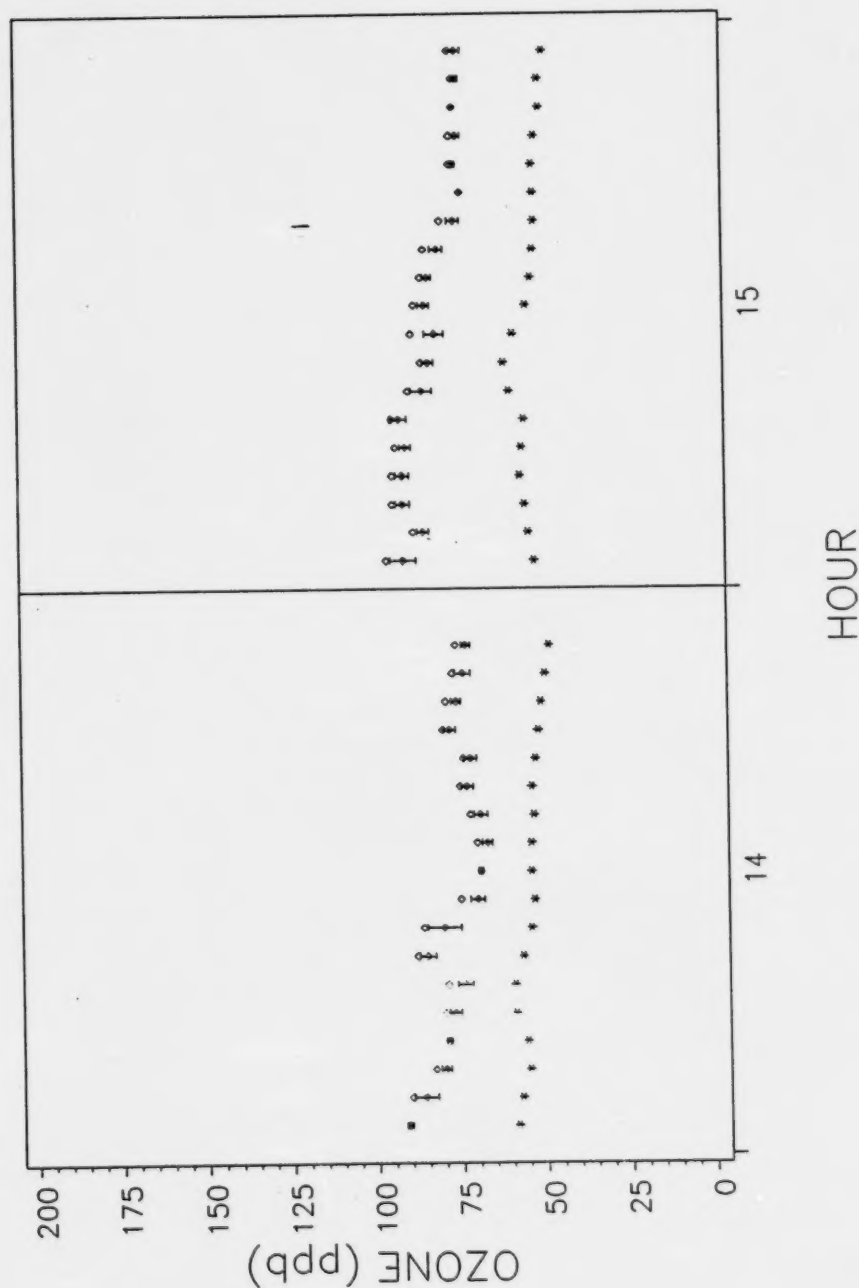


Figure 8.18. Time series of O₃ data from flight on Aug. 8, 1980 from VT to PA. Within each hour period, for each ROM grid cell traversed by the aircraft, the observed mean concentration (diamond) is surrounded by the observed standard deviation with the observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

AIRCRAFT - VT.-N.Y.-PA. (REGIONAL)
 AUGUST 8, 1980 (AV)
 LAYER 2

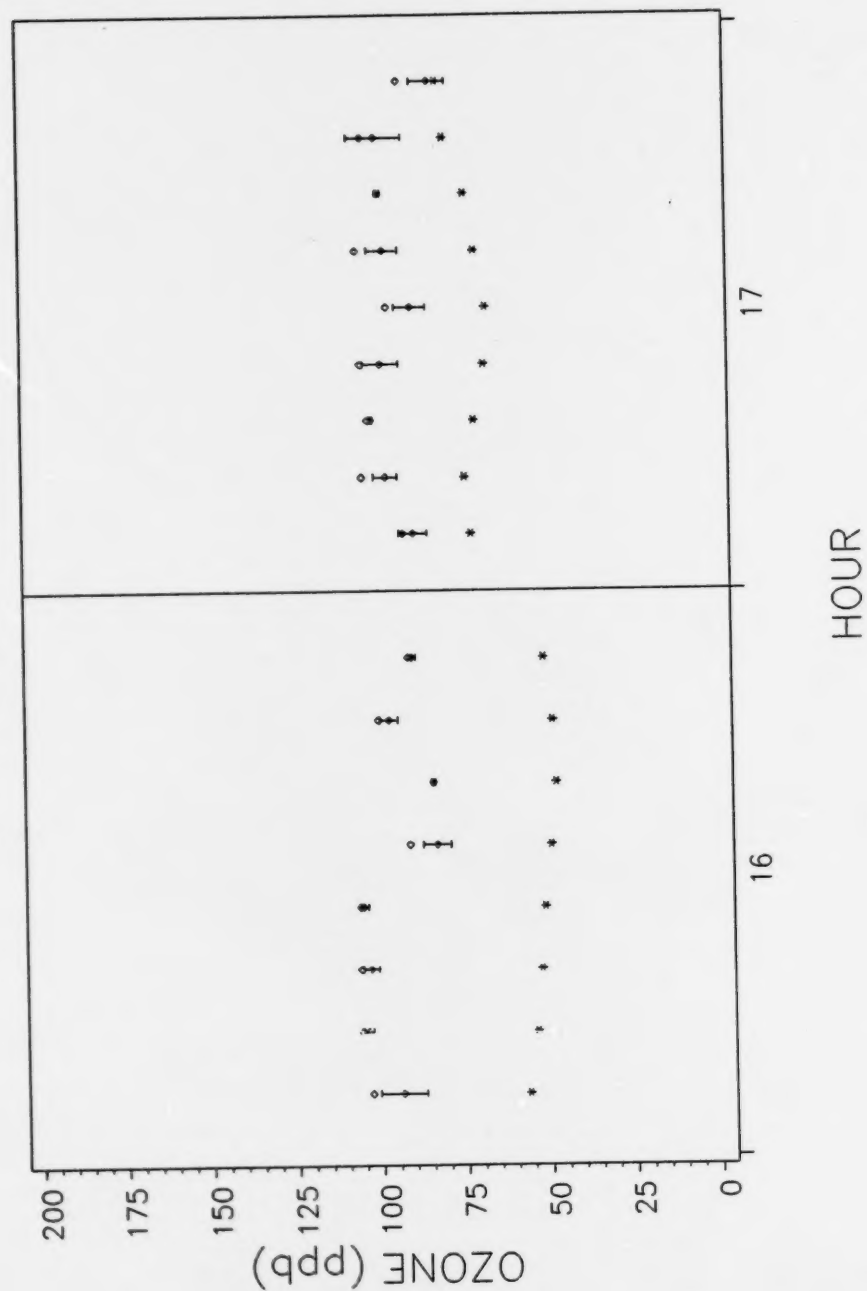


Figure 8.18 (cont.)

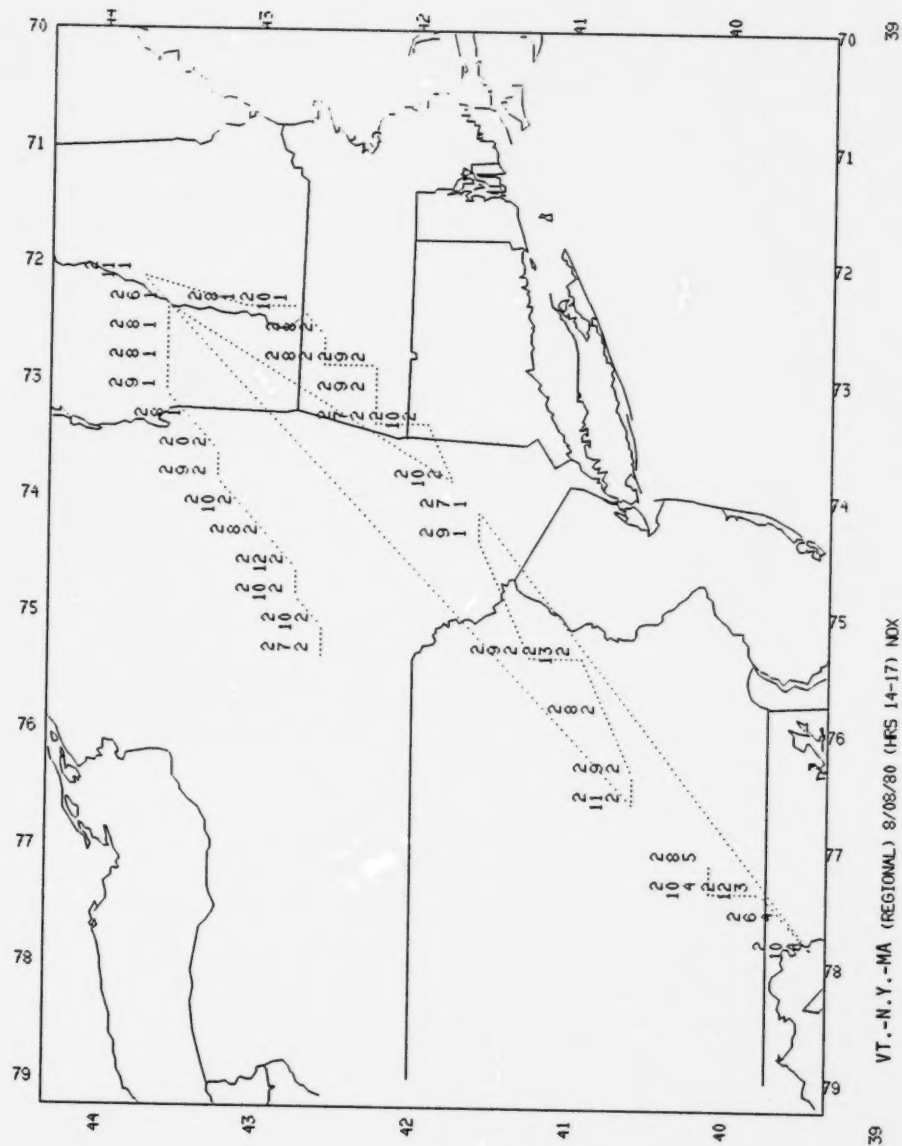


Figure 8.19. Geographical distribution of selected NO_2 data from flight on Aug. 8, 1980 from VT to PA. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - VT.-N.Y.-MA. (REGIONAL)
 AUGUST 8, 1980 (AV)
 LAYER 2

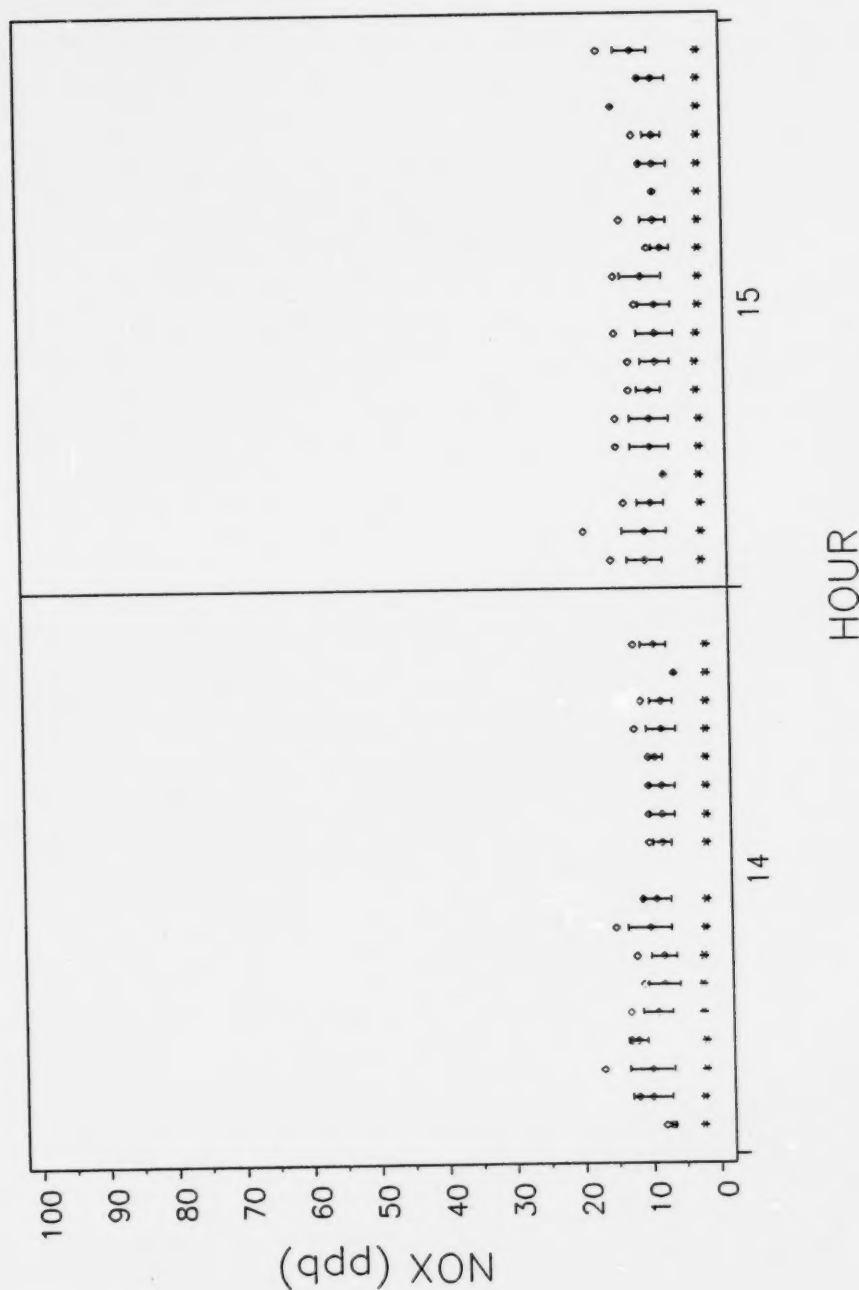


Figure 8.20. Time series of NO_x data from flight on Aug. 8, 1980 from VT to PA. Within each hour period, for each ROM grid cell traversed by the aircraft, the observed mean concentration (diamond) is surrounded by the observed standard deviation with the observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

AIRCRAFT - VT.-N.Y.-MA. (REGIONAL)
 AUGUST 8, 1980 (AV)
 LAYER 2

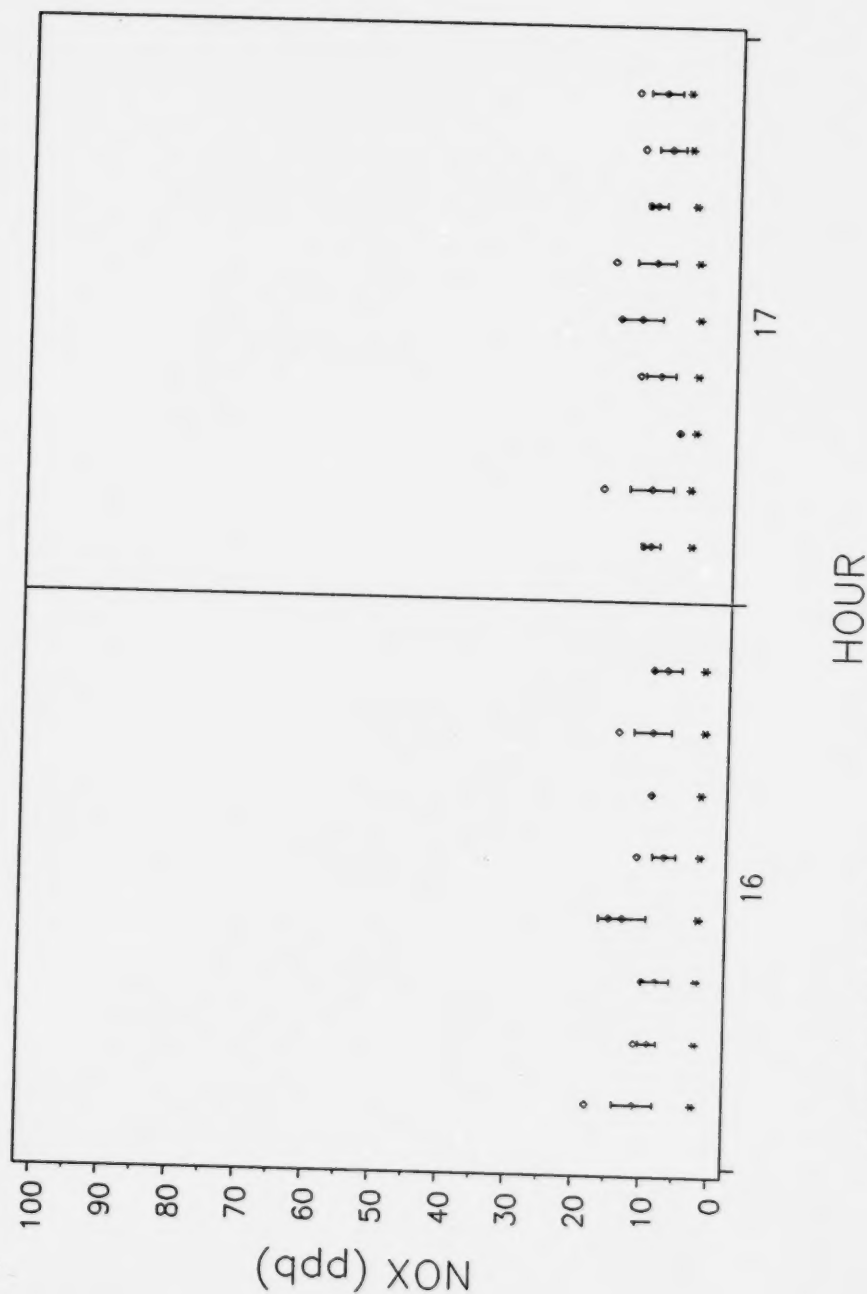


Figure 8.20 (cont.)

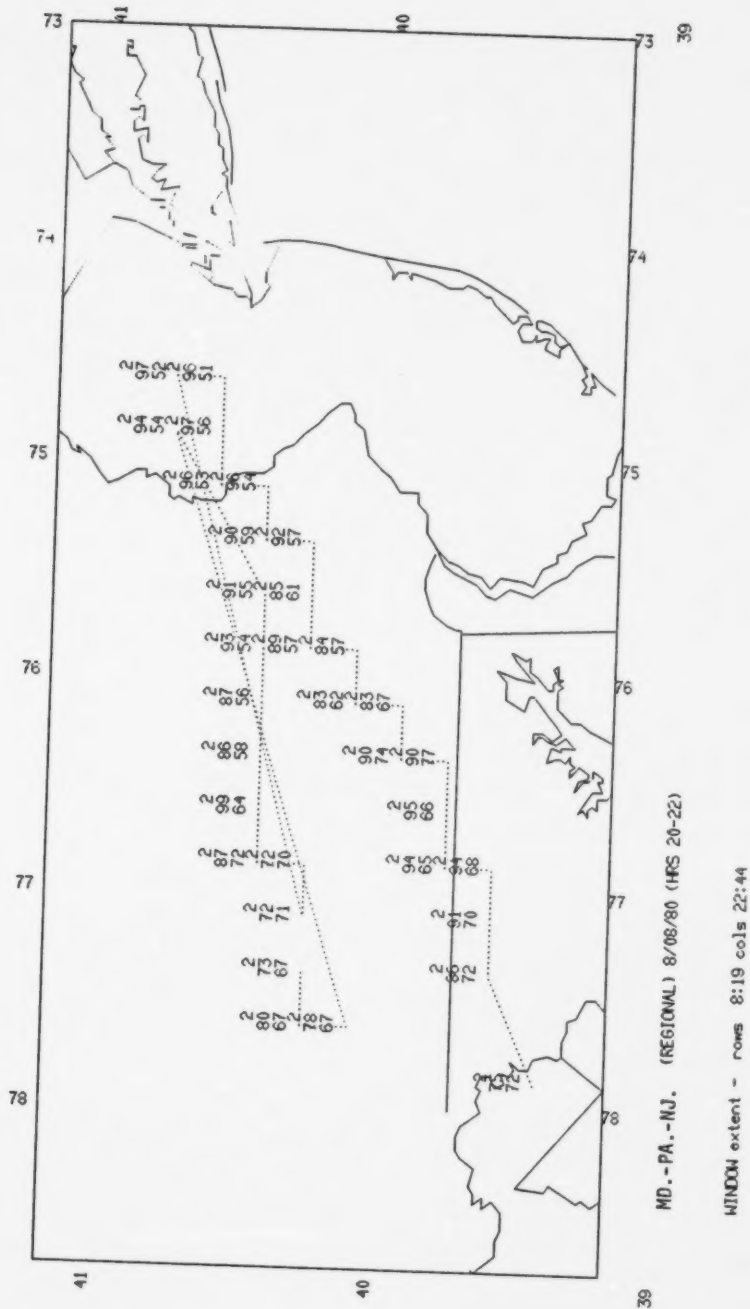


Figure 8.21. Geographical distribution of selected O_3 data from flight on Aug. 8, 1980 from MD to NJ. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - MD-PA-NJ. (REGIONAL)
 AUGUST 8, 1980 (AV)
 LAYER 2

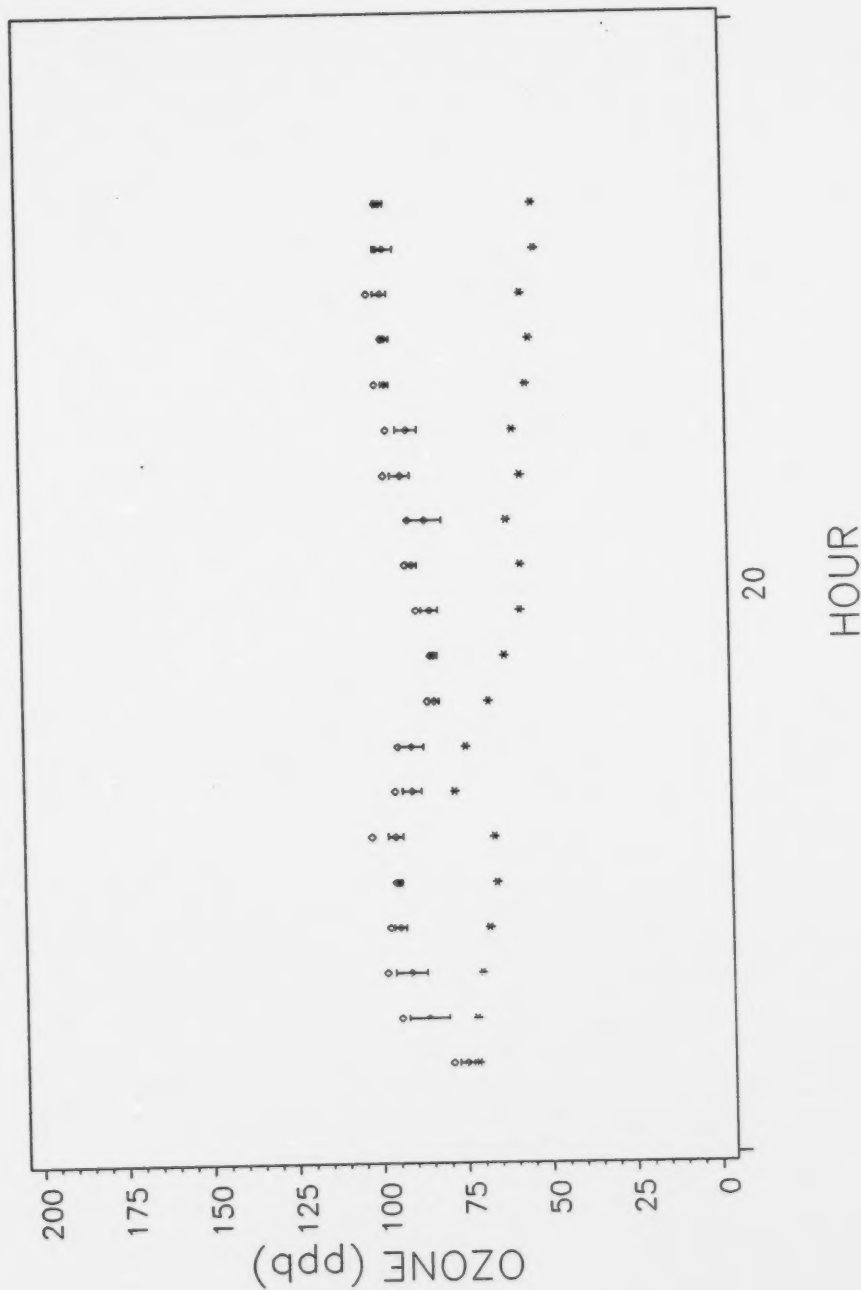


Figure 8.22. Time series of O₃ data from flight on Aug. 8, 1980 from MD to NJ. Within each hour period, for each ROM grid cell traversed by the aircraft, the observed mean concentration (diamond) is surrounded by the observed standard deviation with the observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

AIRCRAFT — MD.-PA.-WJ. (REGIONAL)
 AUGUST 8, 1980 (AV)
 LAYER 2

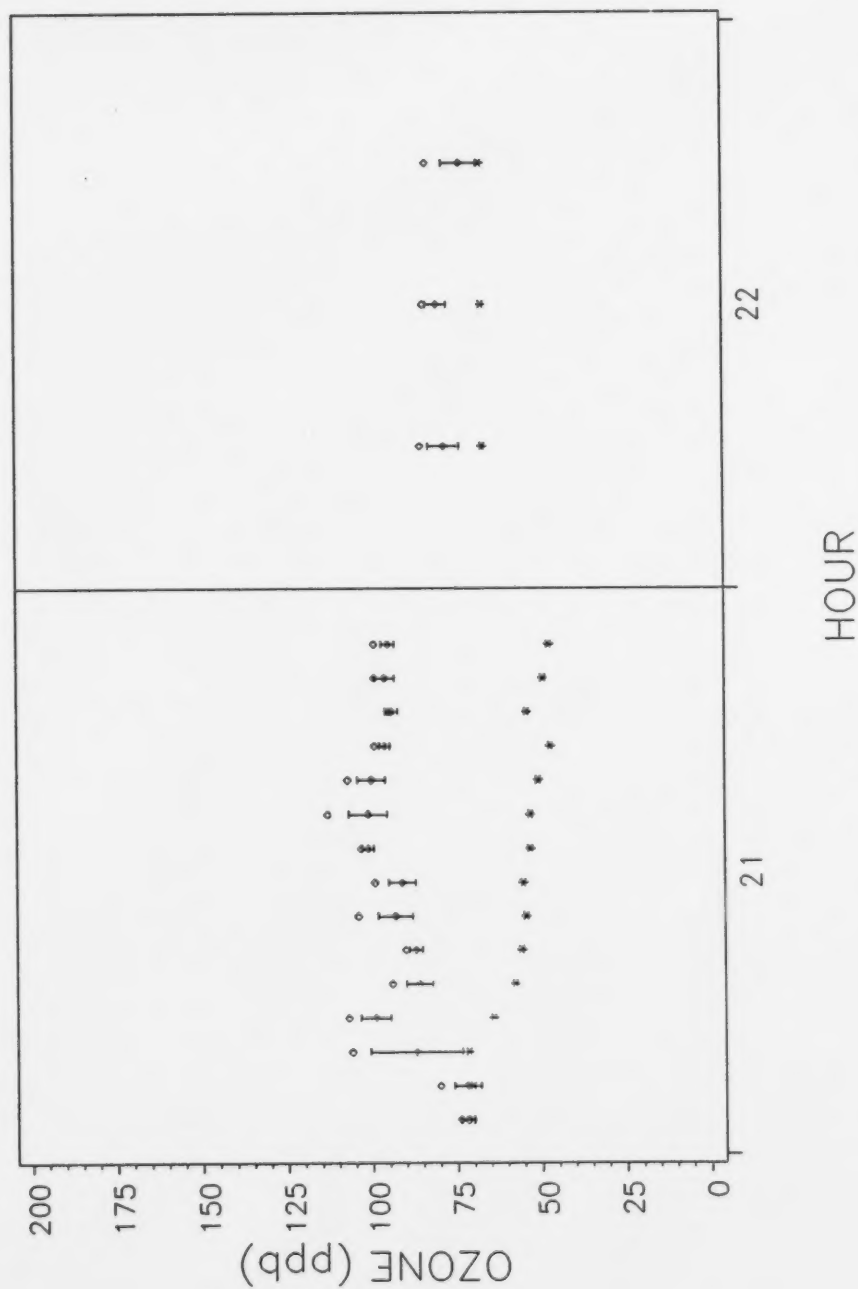


Figure 8.22 (cont.)

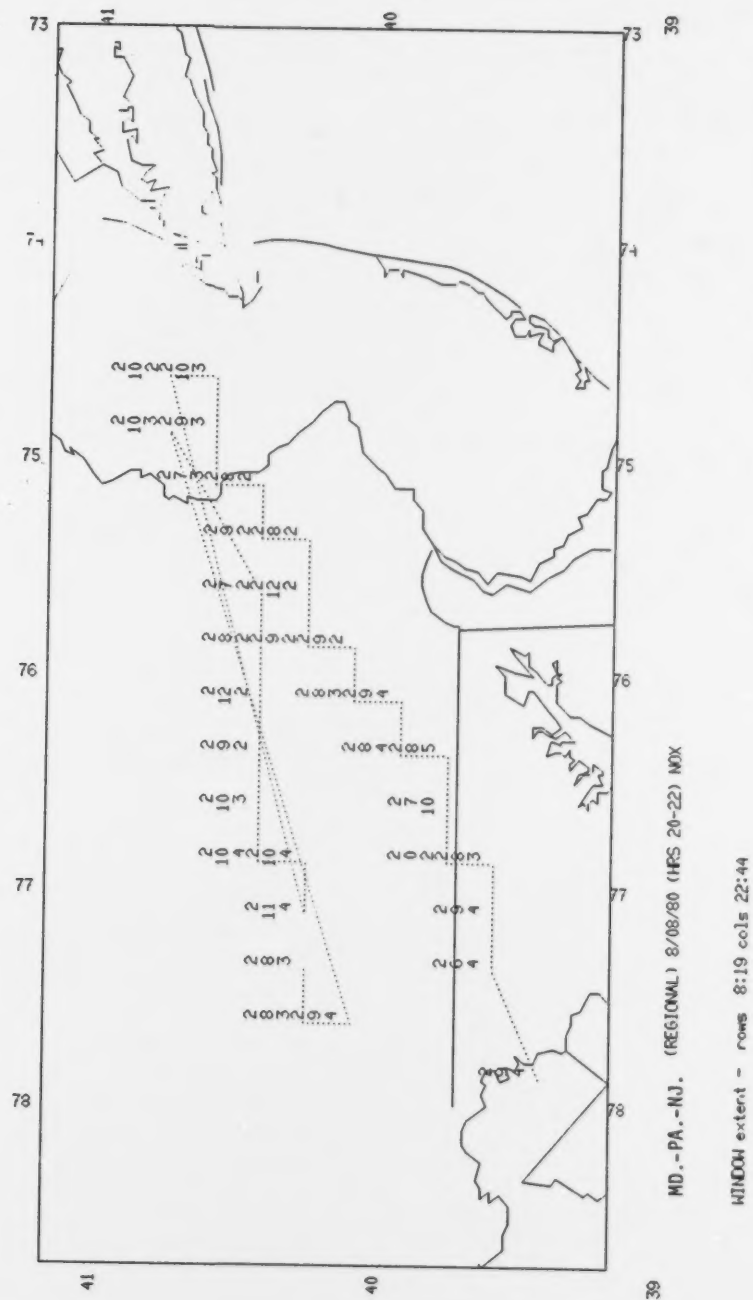


Figure 8.23. Geographical distribution of selected NO_x data from flight on Aug. 8, 1980 from MD to NJ. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - MD.-PA.-NJ. (REGIONAL)
 AUGUST 8, 1980 (AV)
 LAYER 2

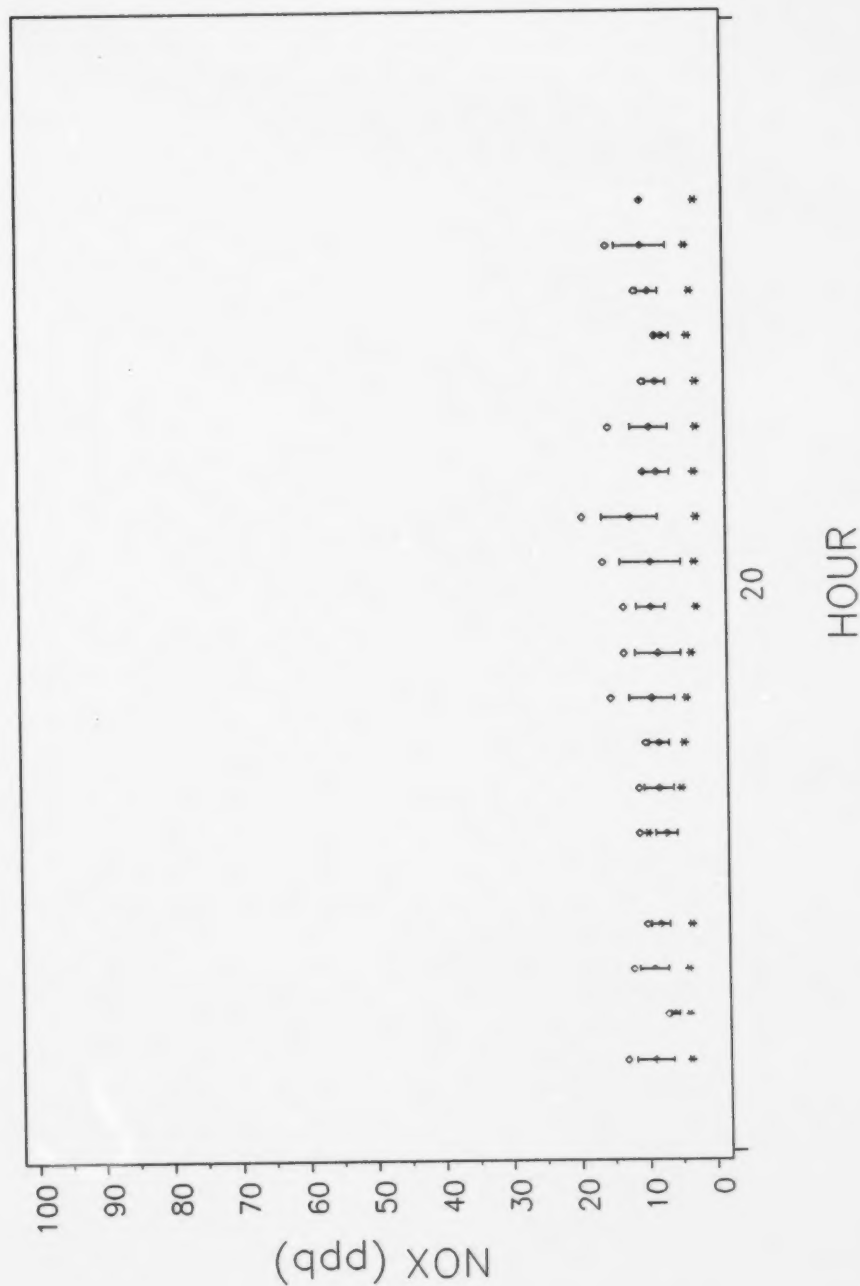


Figure 8.24. Time series of NO_x data from flight on Aug. 8, 1980 from MD to NJ. Within each hour period, for each ROM grid cell traversed by the aircraft, the observed mean concentration (diamond) is surrounded by the observed standard deviation with the observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

AIRCRAFT - MD-PA-JJ. (REGIONAL)
 AUGUST 8, 1980 (AV)
 LAYER 2

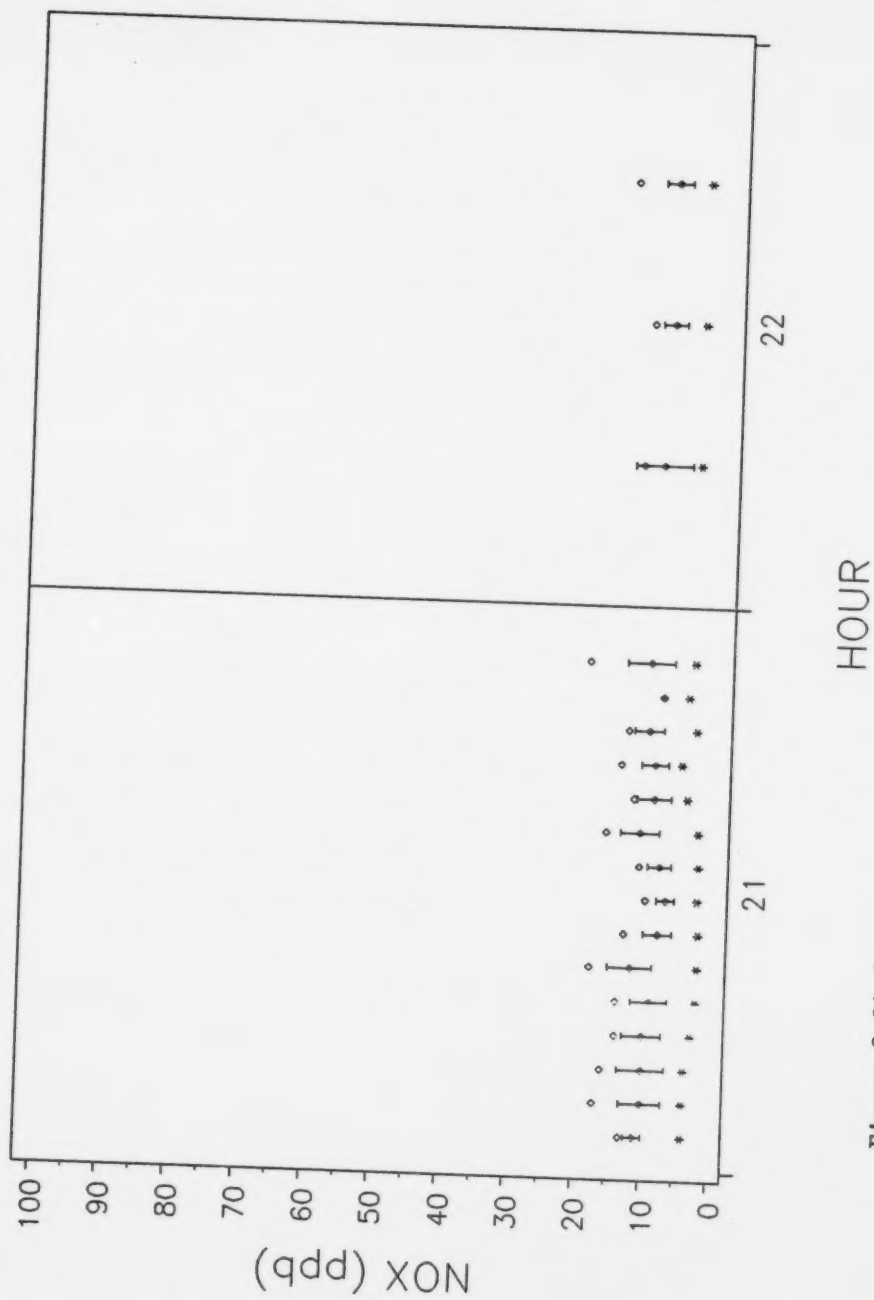
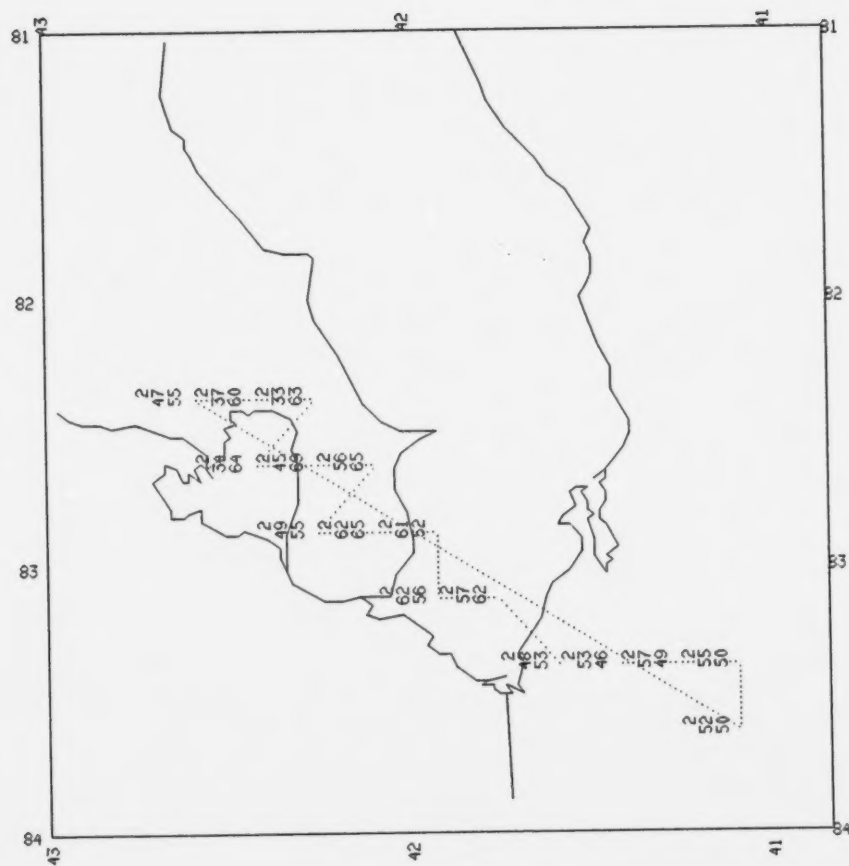


Figure 8.24 (cont.)



OHIO-MICH. (REGIONAL) 8/15/80 (HRS 11-13)

WINDOW extent - rows 18:30 cols 1:12

Figure 8.25. Geographical distribution of selected O₃ data from flight on Aug. 15, 1980 from OH to MI. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - OHIO-MI. (REGIONAL)
AUGUST 15, 1980 (AV)
LAYER 2

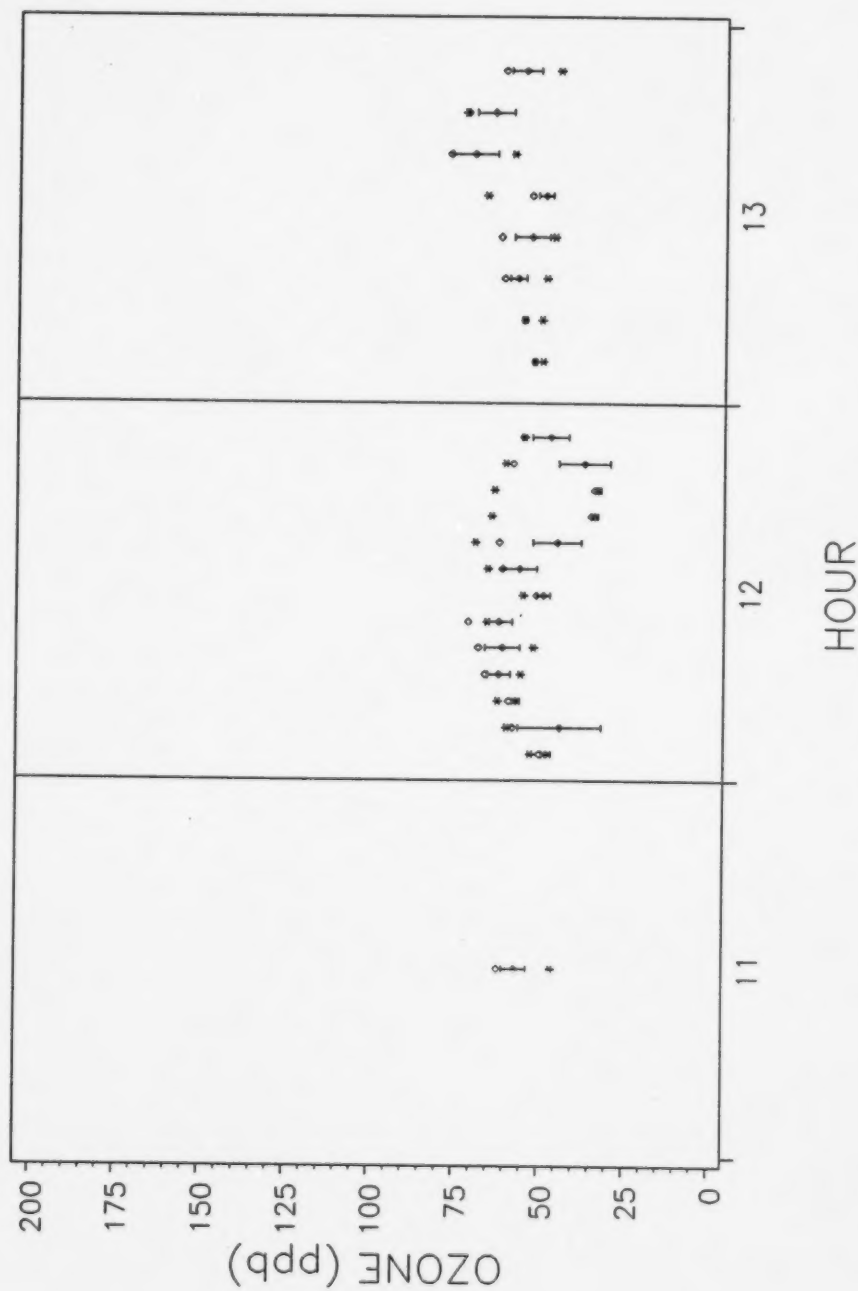


Figure 8.26. Time series of O₃ data from flight on Aug. 15, 1980 from OH to MI. Within each hour period, for each ROM grid cell traversed by the aircraft, the observed mean concentration (diamond) is surrounded by the observed standard deviation with the observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

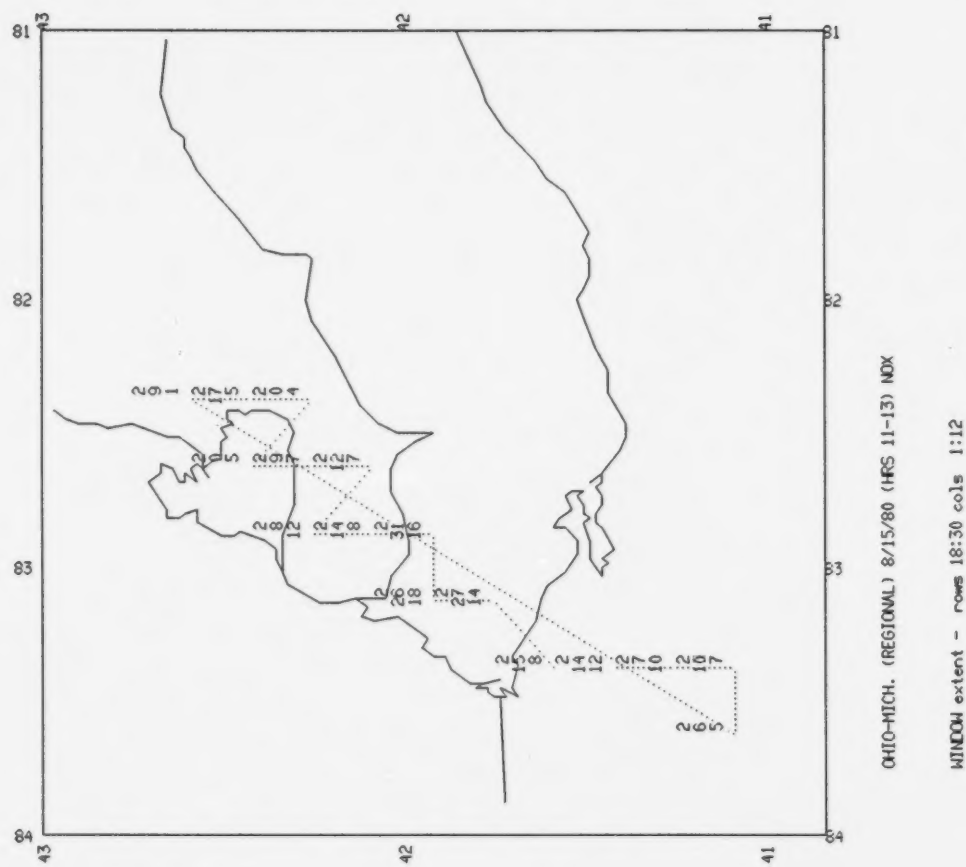


Figure 8.27. Geographical distribution of selected NO_x data from flight on Aug. 15, 1980 from OH to MI. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - OHIO-MI. (REGIONAL)
AUGUST 15, 1980 (AV)
LAYER 2

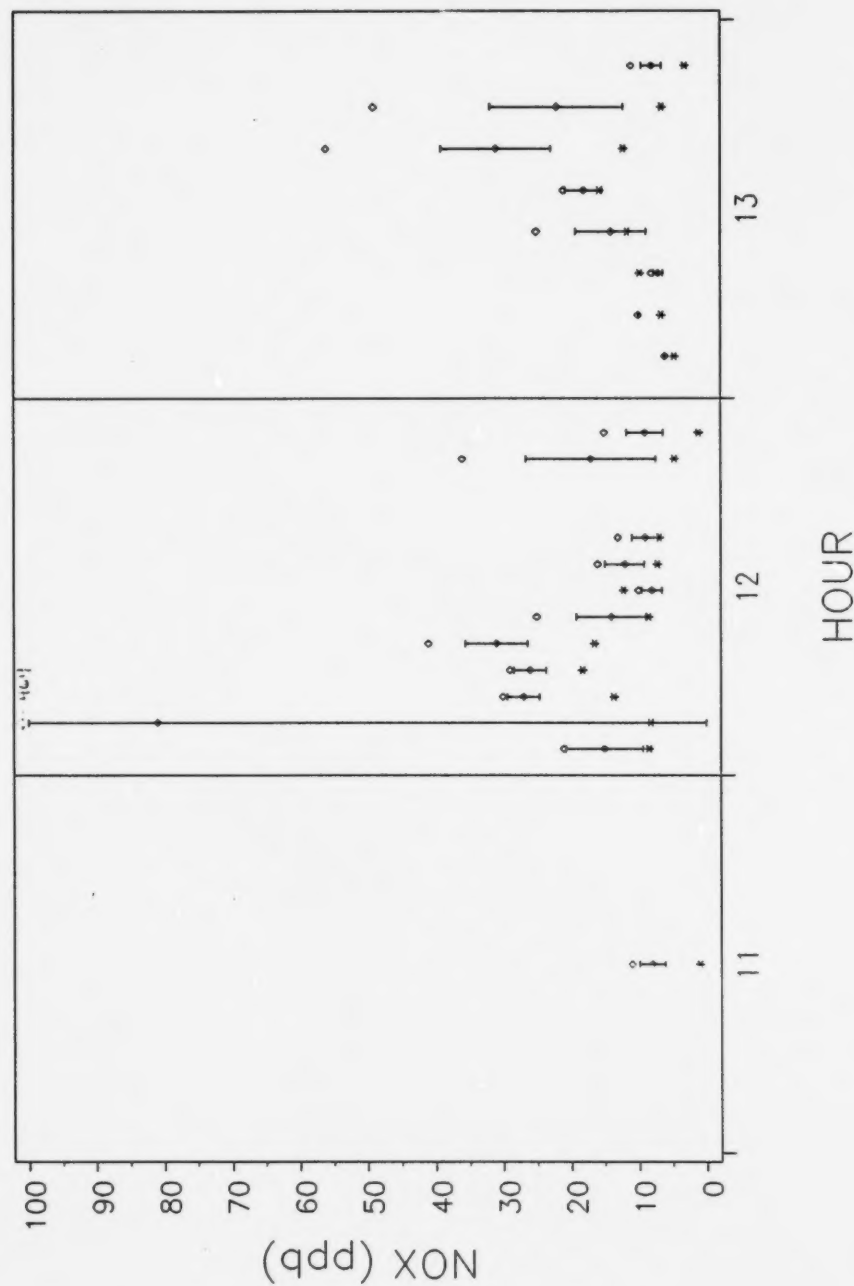


Figure 8.28. Time series of NO_x data from flight on Aug. 15, 1980 from OH to MI. Within each hour period, for each ROM grid cell traversed by the aircraft, the observed mean concentration (diamond) is surrounded by the observed standard deviation with the observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

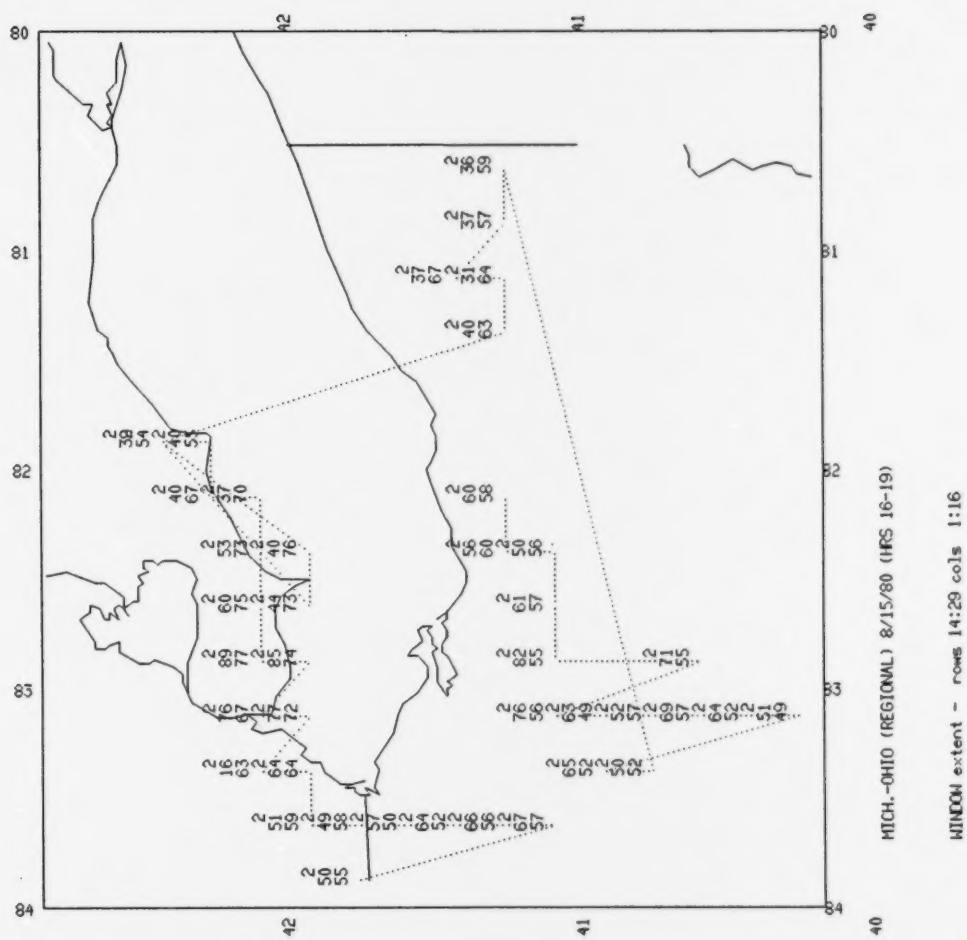


Figure 8.29. Geographical distribution of selected O_3 data from flight on Aug. 15, 1980 from MI to OH. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - MI.-OHIO (REGIONAL)
AUGUST 15, 1980 (AV)
LAYER 2

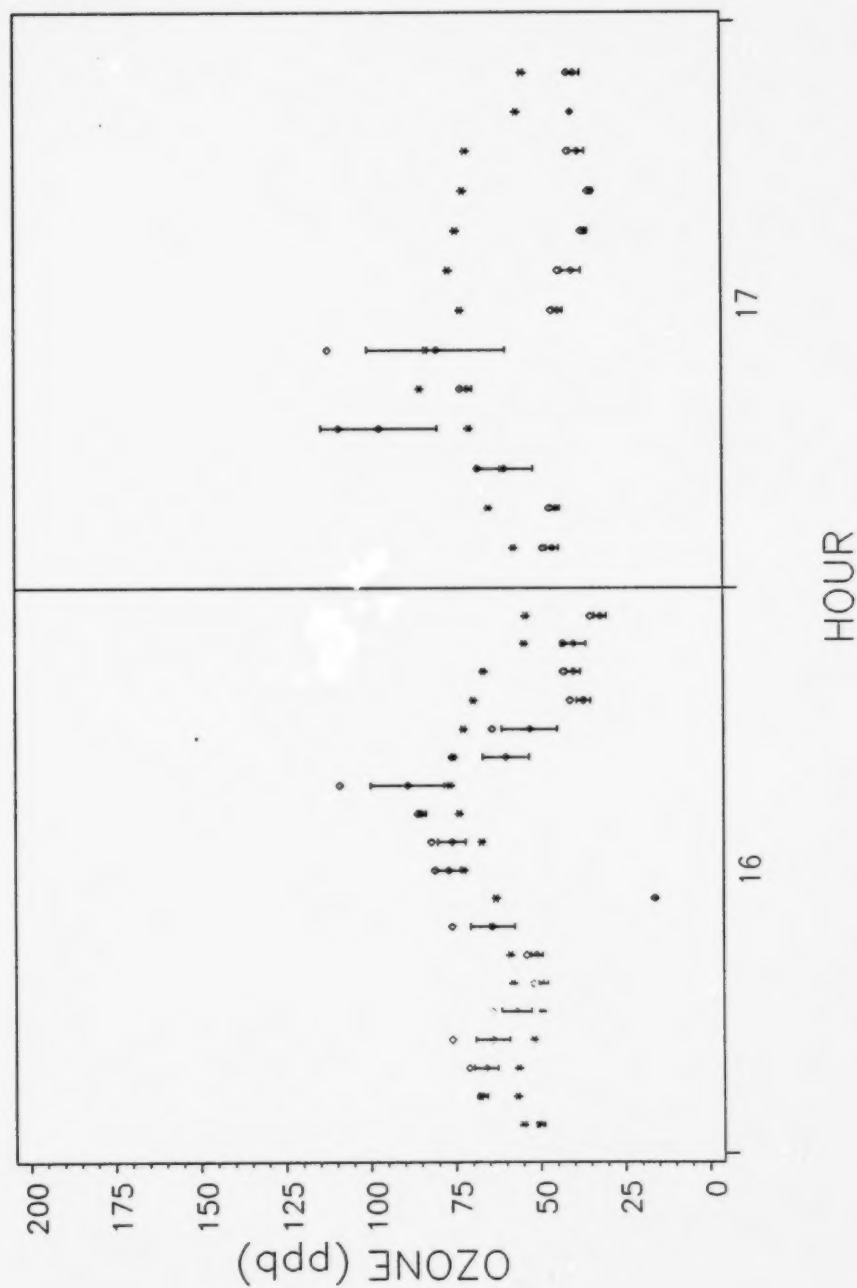


Figure 8.30. Time series of O₃ data from flight on Aug. 15, 1980 from MI to OH. Within each hour period, for each ROM grid cell traversed by the aircraft, the observed mean concentration (diamond) is surrounded by the observed standard deviation with the observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

AIRCRAFT - MI.-OHIO (REGIONAL)
AUGUST 15, 1980 (AV)
LAYER 2

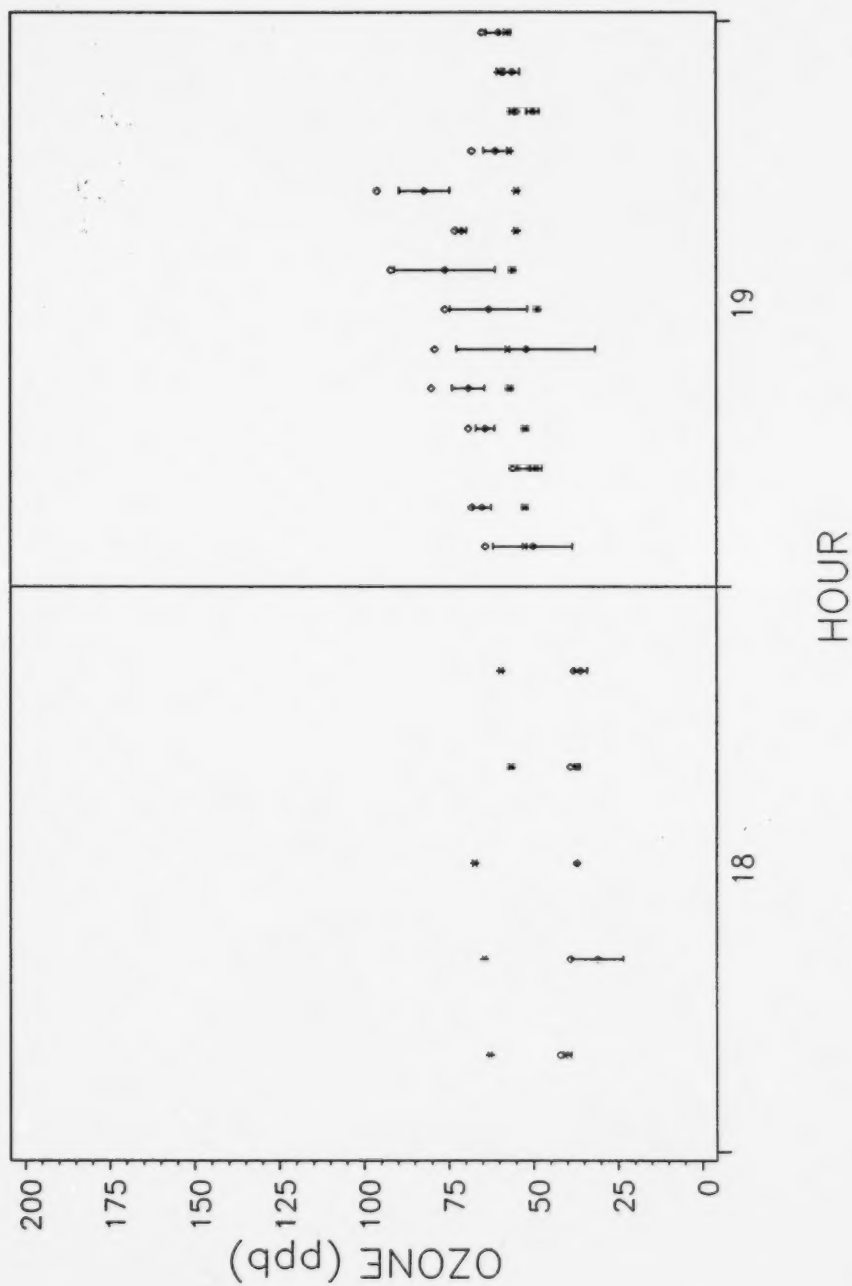


Figure 8.30 (cont.)

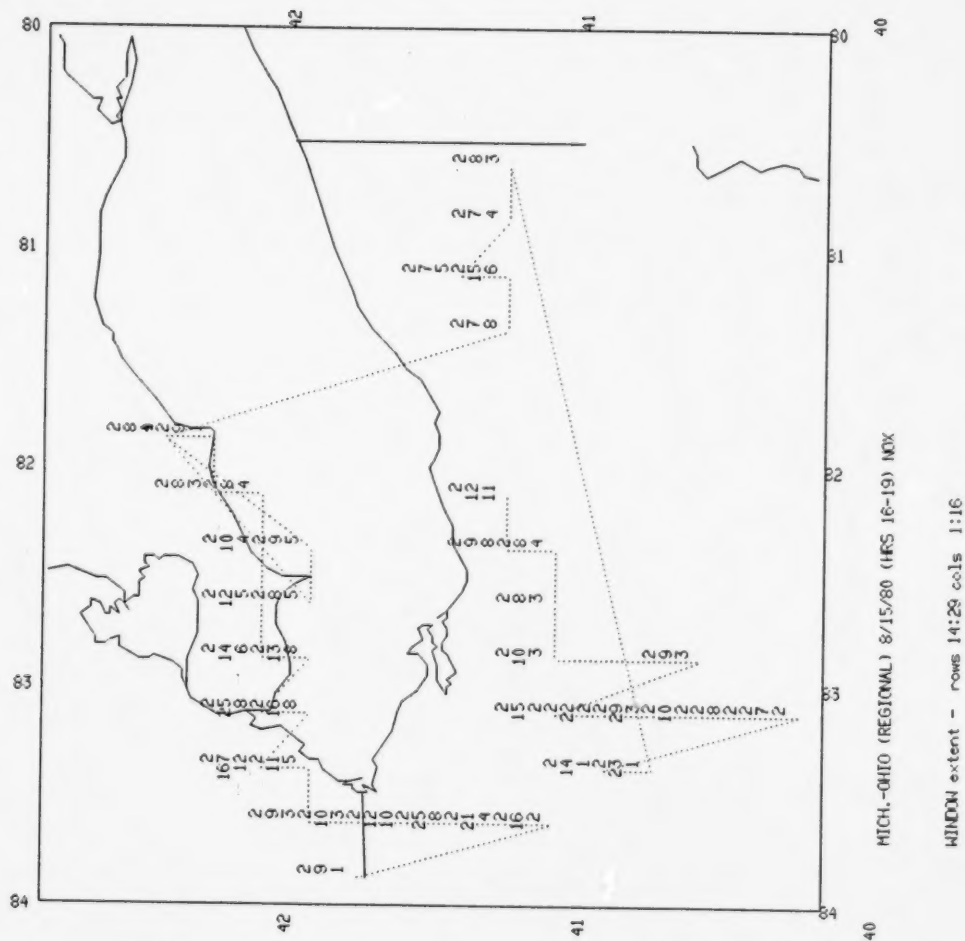


Figure 8.31. Geographical distribution of selected NO_x data from flight on Aug. 15, 1980 from MI to OH. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - MI.-OHIO (REGIONAL)
AUGUST 15, 1980 (AV)
LAYER 2

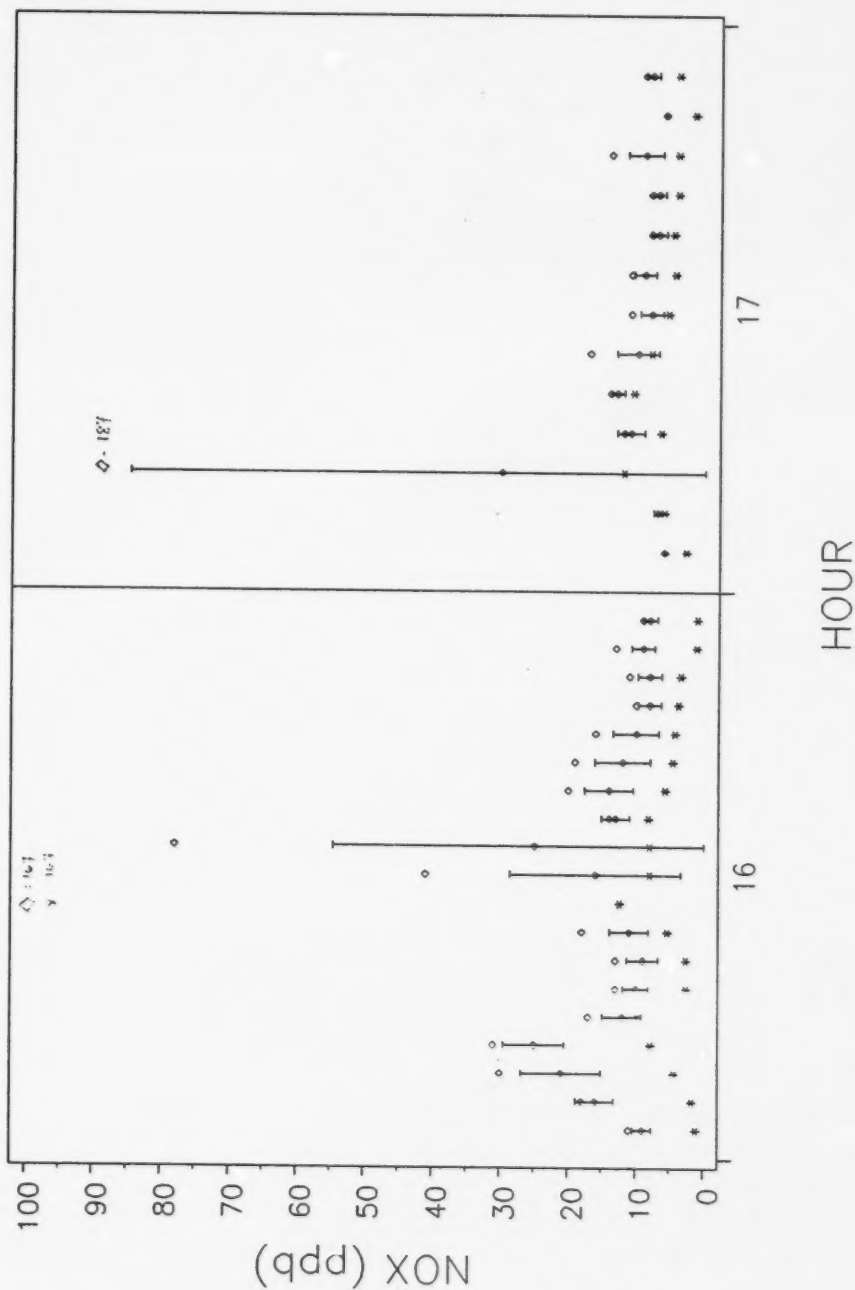


Figure 8.32. Time series of NO_x data from flight on Aug. 15, 1980 from MI to OH. Within each hour period, for each ROM grid cell traversed by the aircraft, the observed mean concentration (diamond) is surrounded by the observed standard deviation with the observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

AIRCRAFT - MI.-OHIO (REGIONAL)
AUGUST 15, 1980 (AV)
LAYER 2

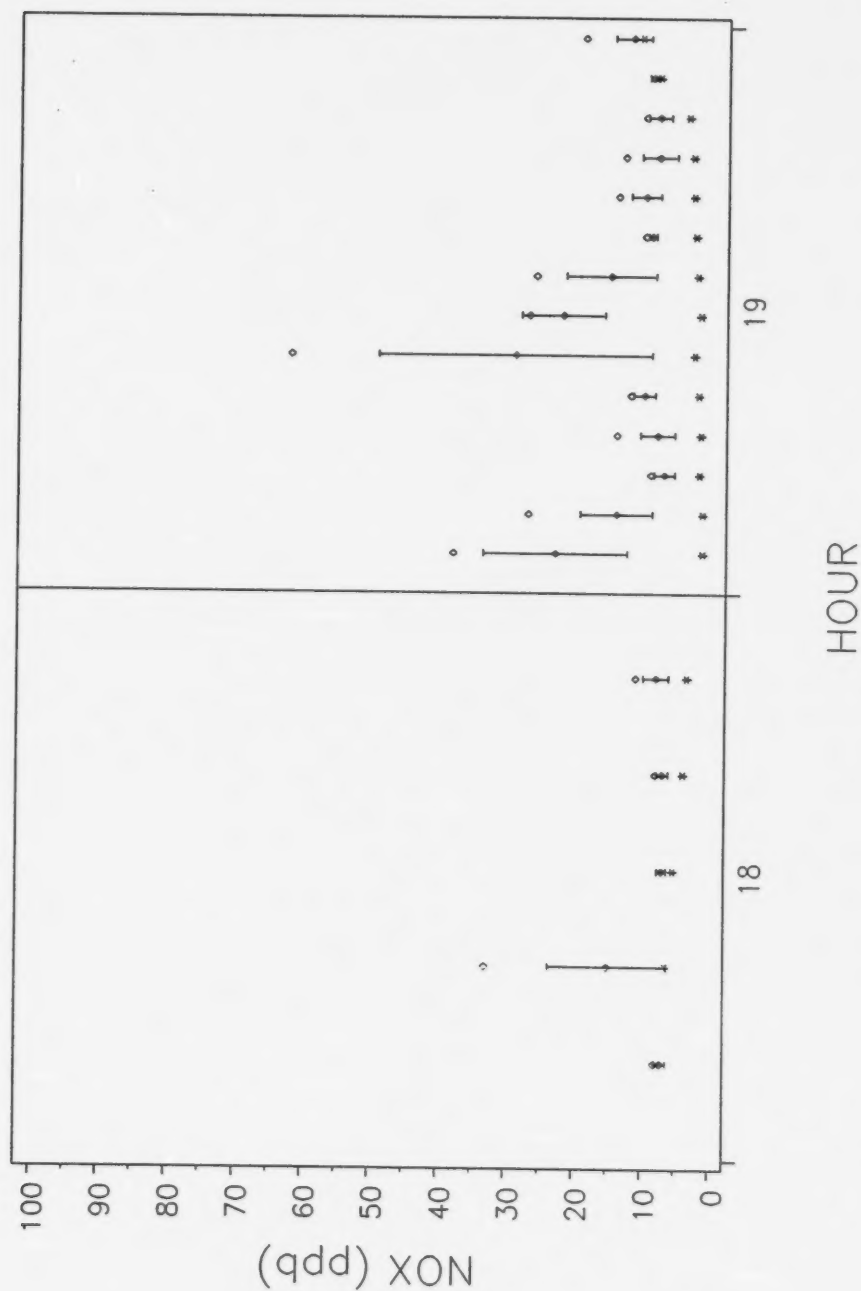
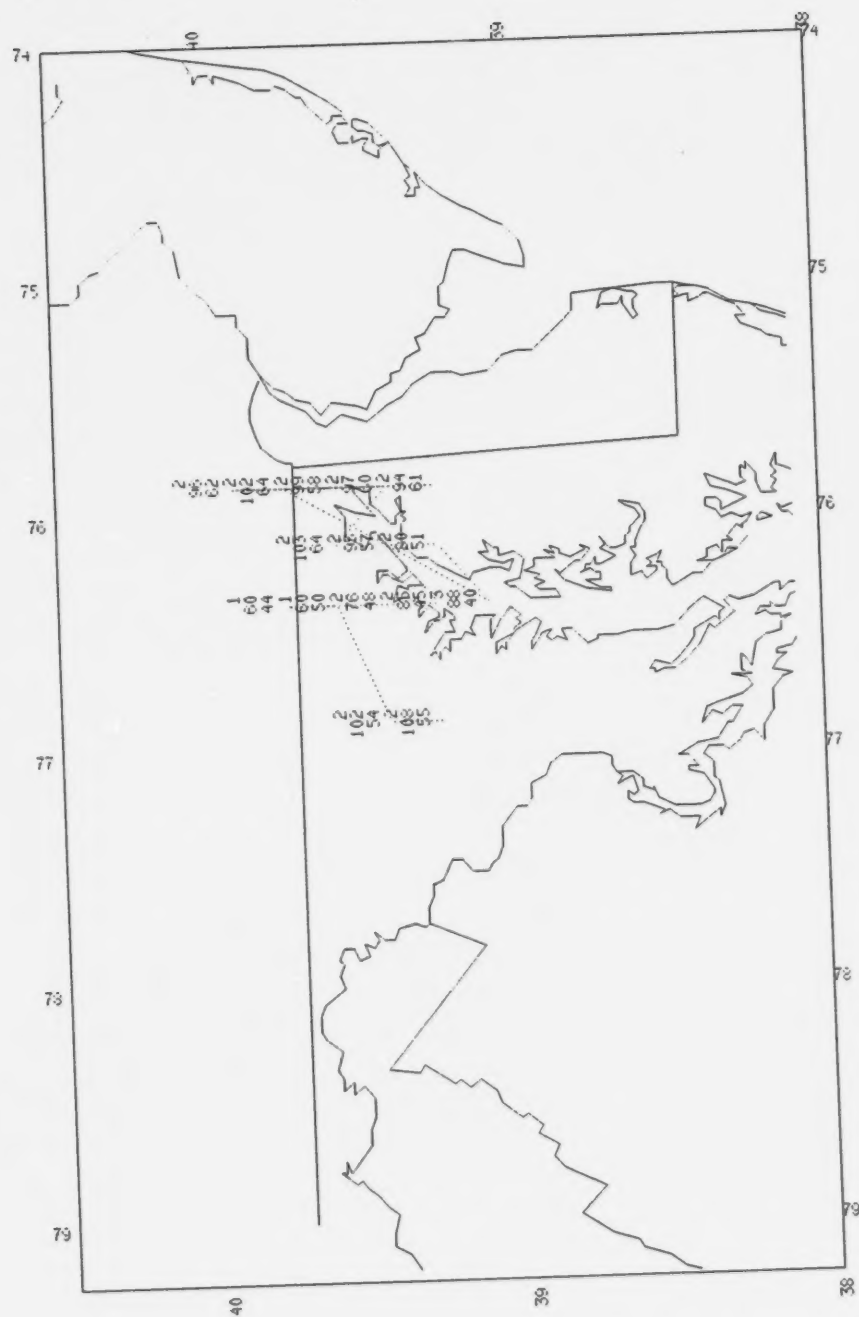


Figure 8.32 (cont.)



BALTIMORE (BAL) 7/16/80 (HRS 6-9)

WINDON extent - rows 1:15 cols 20:40

Figure 8.33. Geographical distribution of selected O₃ data from flight on July 16, 1980 in Baltimore, MD area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - BALTIMORE AREA JULY 16, 1980 (BNL)

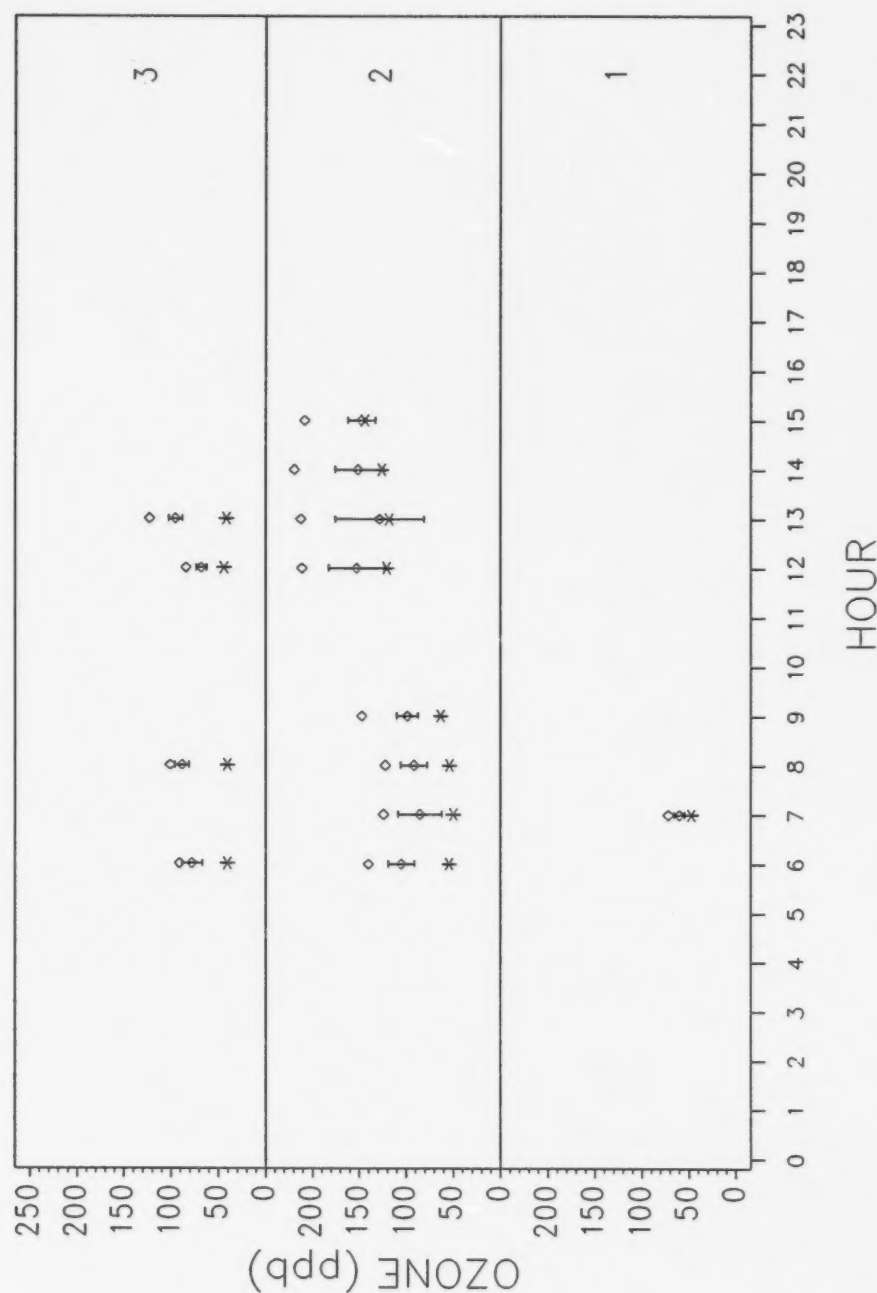


Figure 8.34. Time series of O₃ data from flight on July 16, 1980 in Baltimore, MD area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

AIRCRAFT - BALTIMORE AREA
JULY 16, 1980 (WSU)

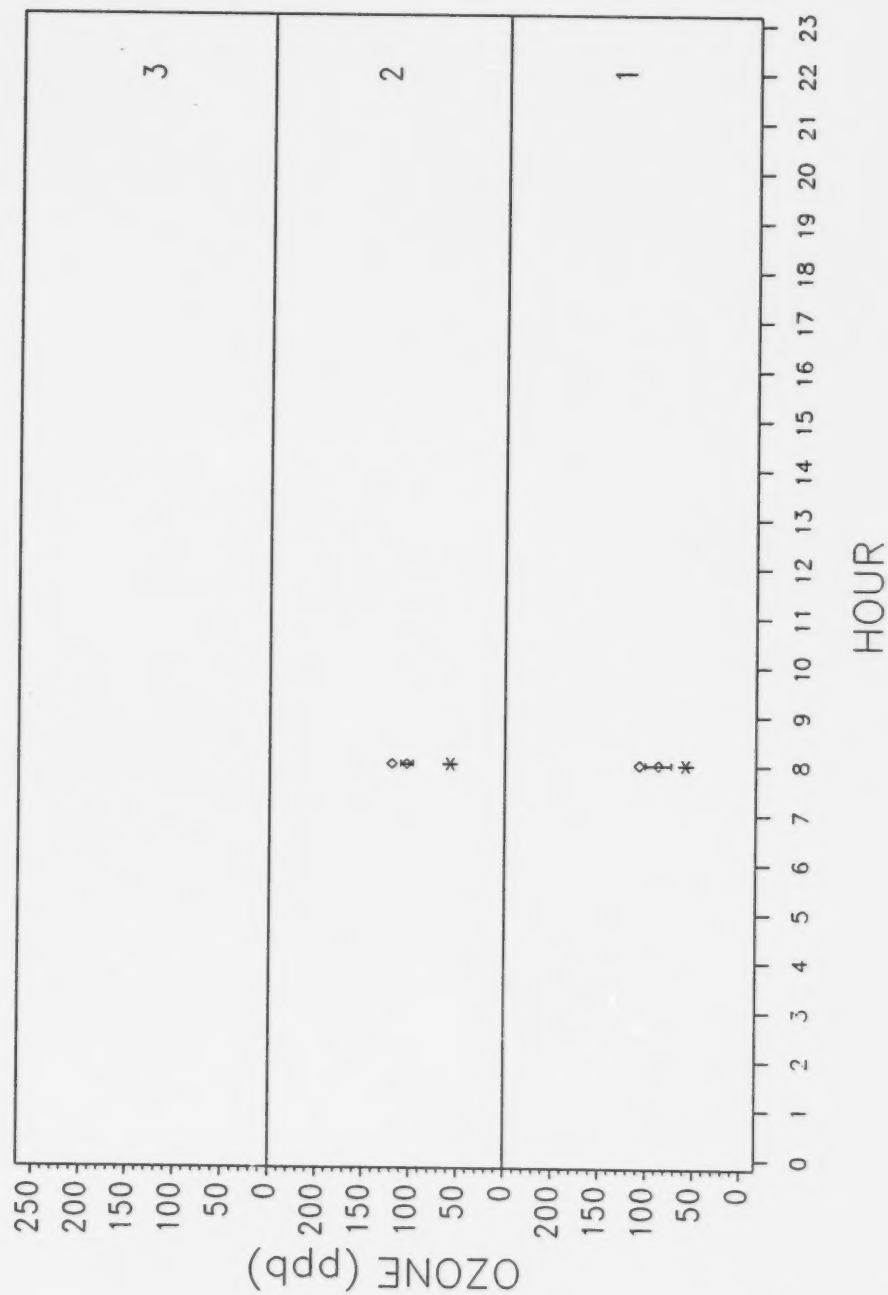
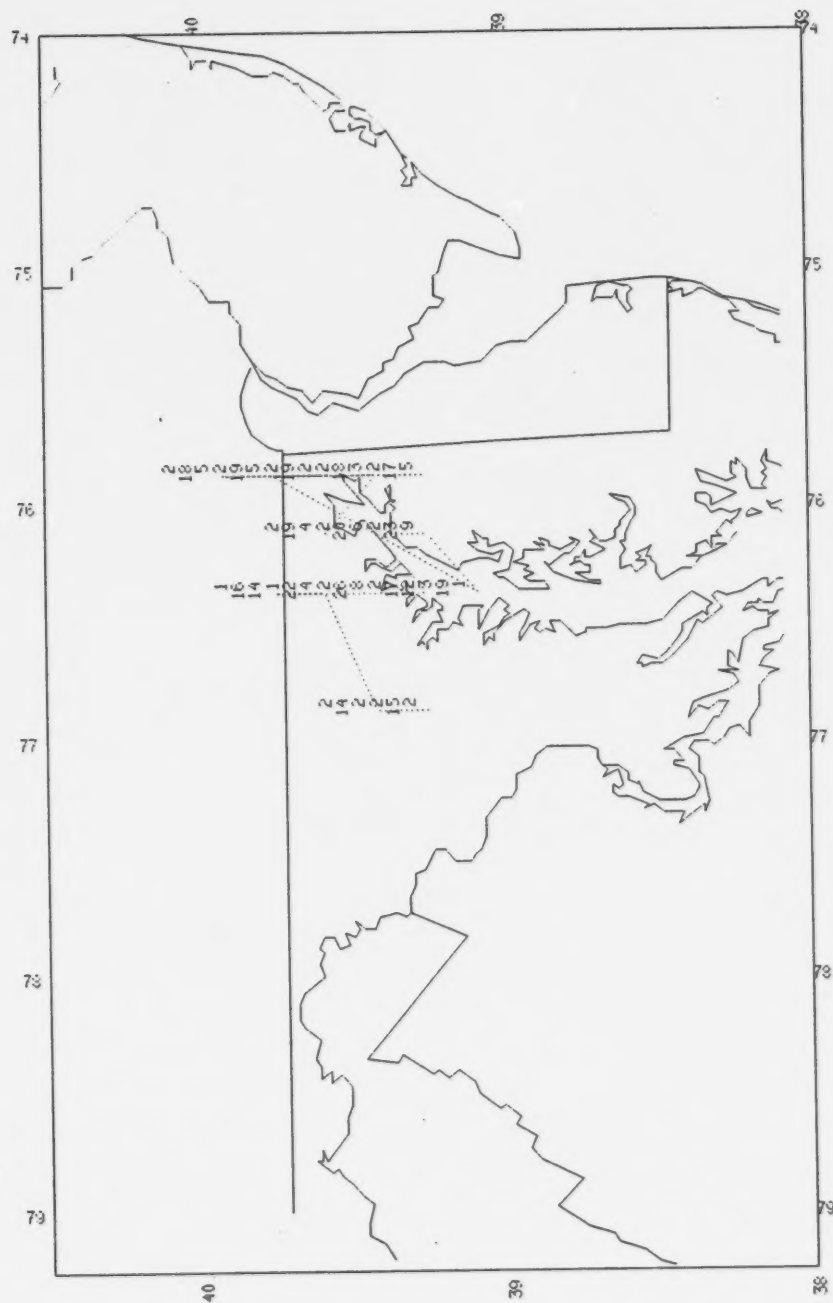


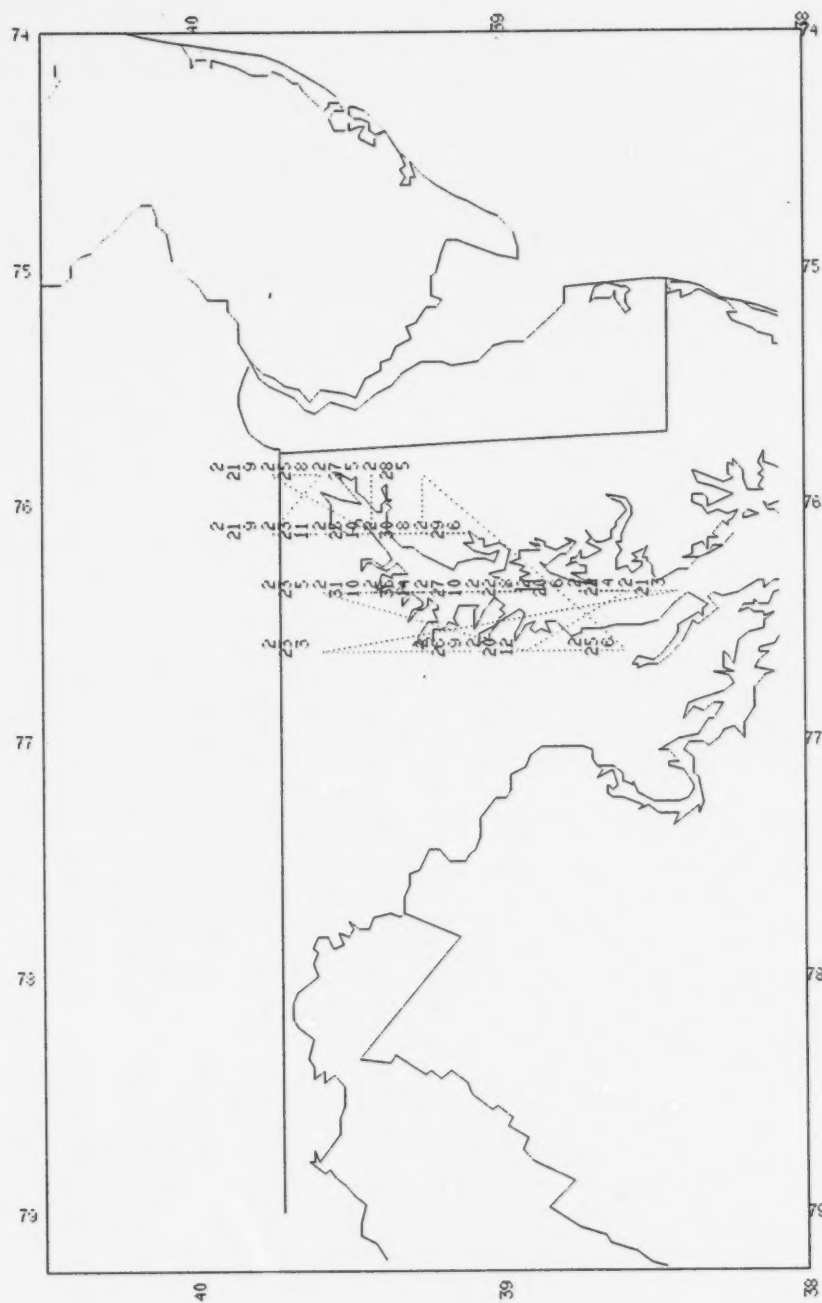
Figure 8.34 (cont.)



BALTIMORE (BIL) 7/16/80 (HRS 6-9) MIX

WINDW extent - rows 1:15 cols 20:40

Figure 8.35. Geographical distribution of selected NO_x data from flight on July 16, 1980 in Baltimore, MD area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).



BALTIMORE (PA) 7/16/80 (HRS 12-15) NOX

HINDO4 extent - rows 1:15 cols 20:40

Figure 8.35 (cont.)

AIRCRAFT - BALTIMORE AREA JULY 16, 1980 (BNL)

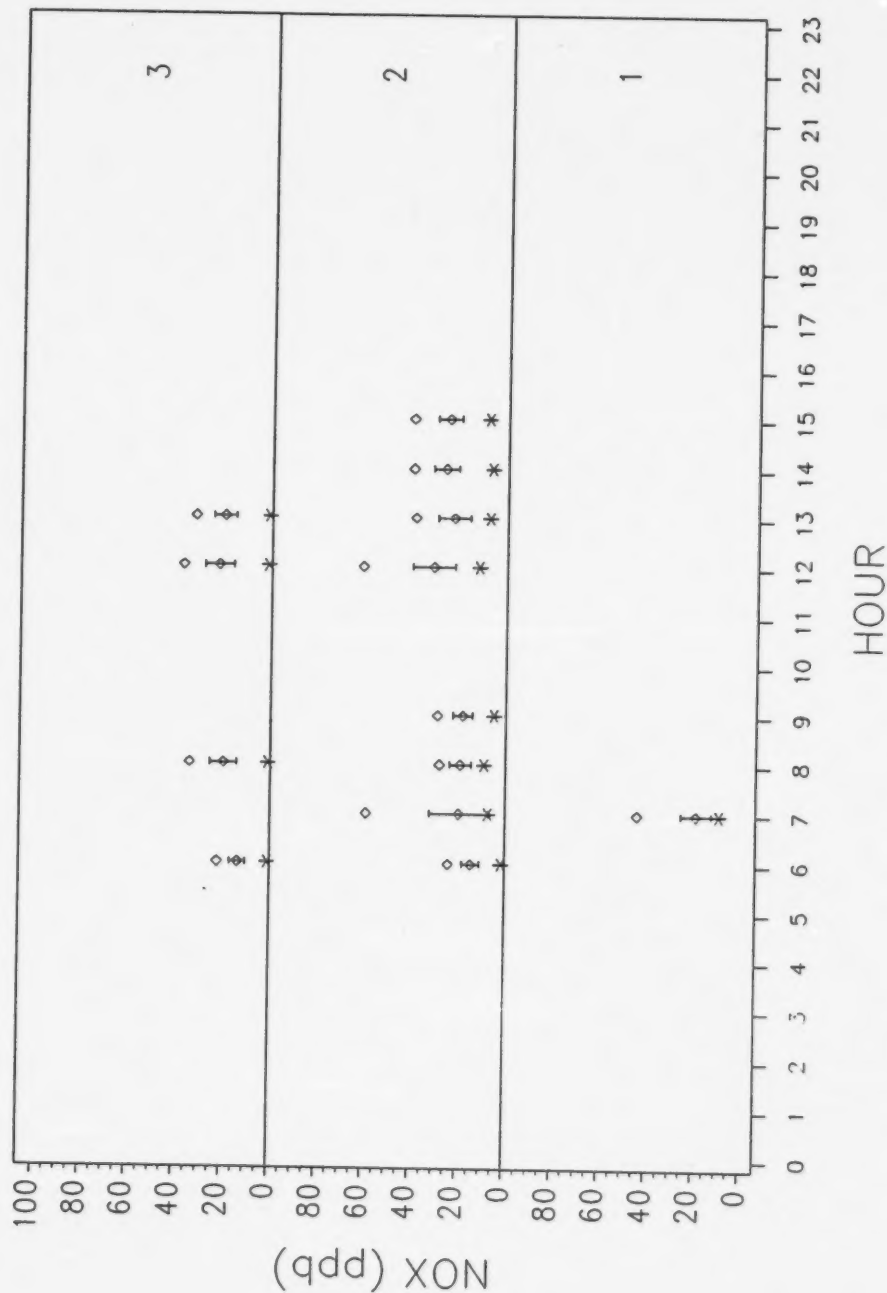


Figure 8.36. Time series of NO_x data from flight on July 16, 1980 in Baltimore, MD area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

AIRCRAFT - BALTIMORE AREA
JULY 16, 1980 (WSU)

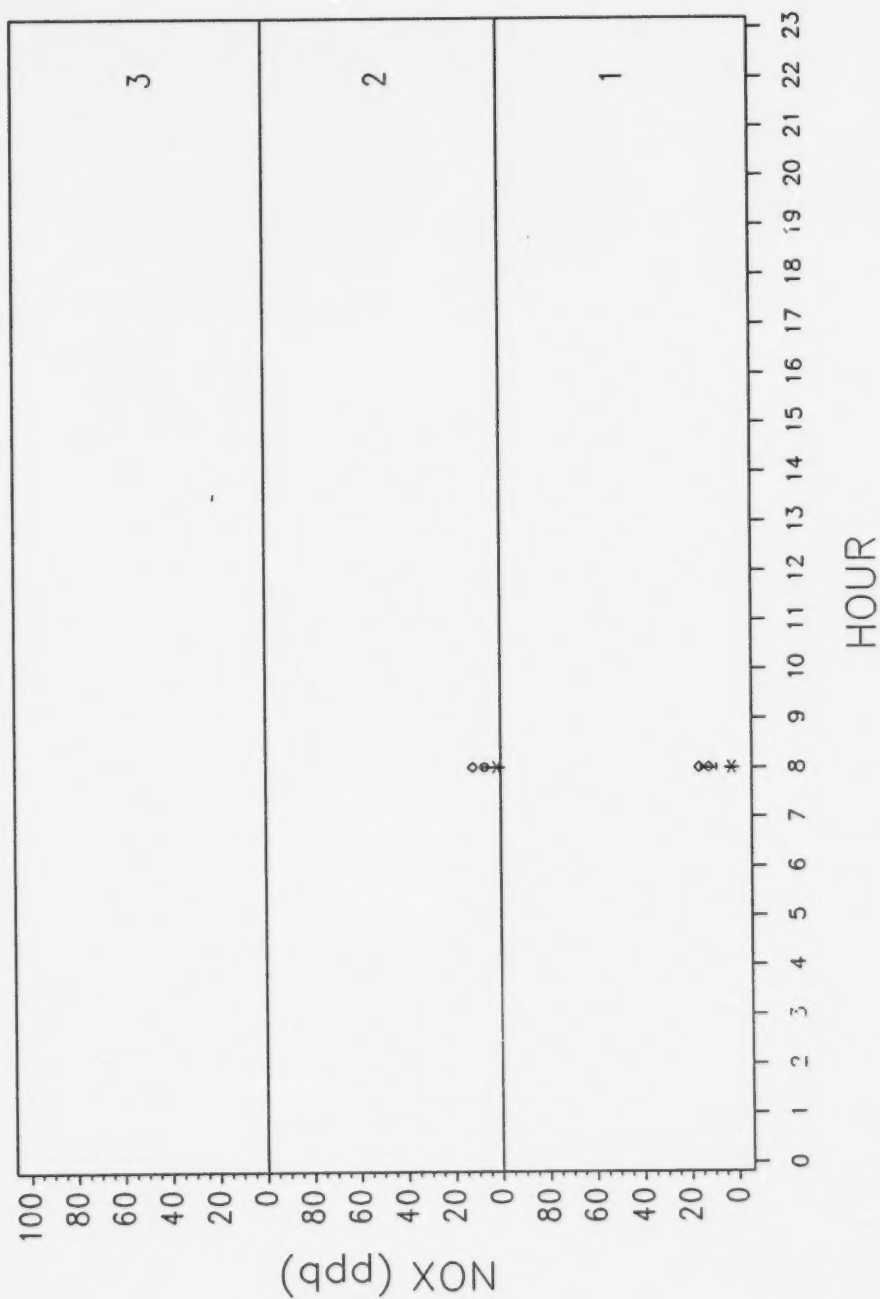
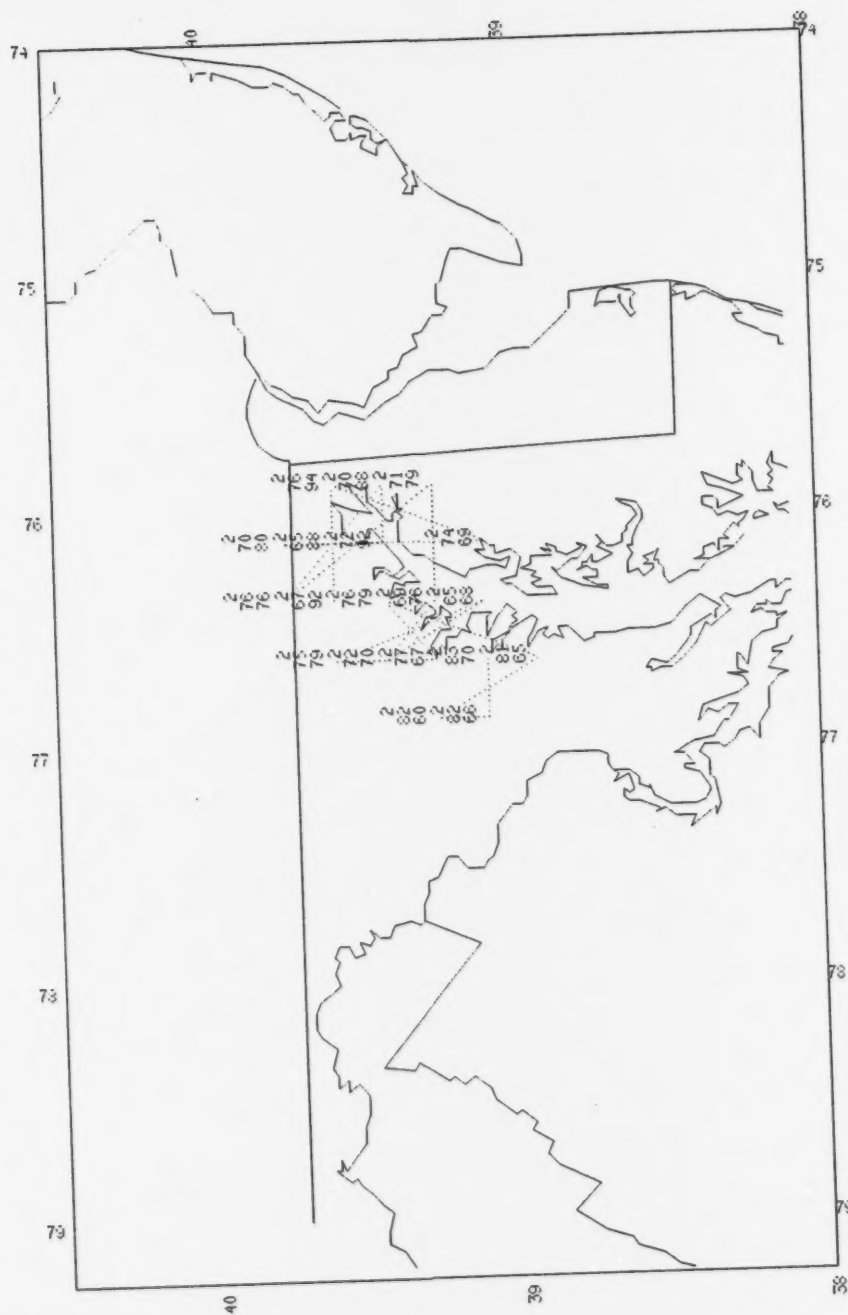


Figure 8.36 (cont.)



BALTIMORE (BAL) 7/19/80 (HRS 6-9)

MINIMUM extent - rows 1:15 cols 20:40

Figure 8.37. Geographical distribution of selected O₃ data from flight on July 19, 1980 in Baltimore, MD area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

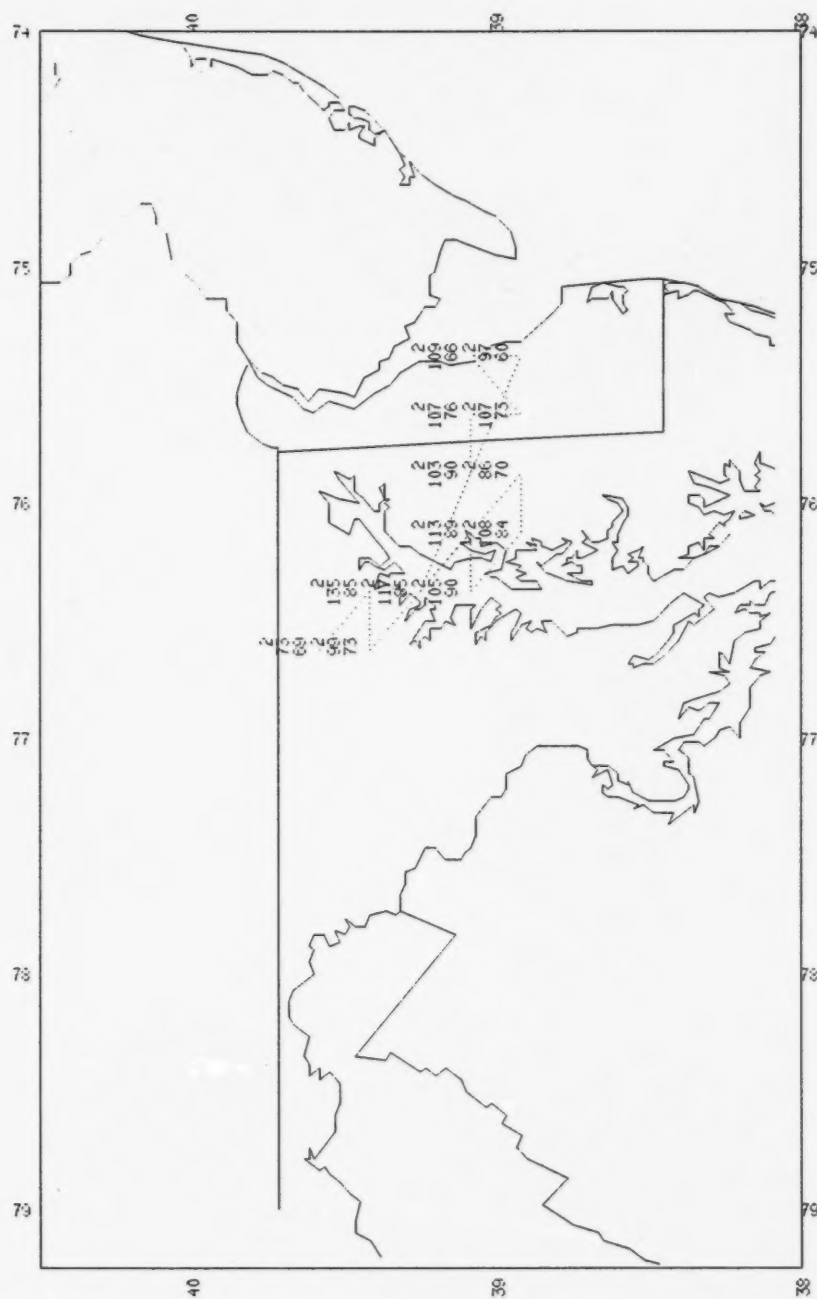


Figure 8.37 (cont.)

AIRCRAFT - BALTIMORE AREA JULY 19, 1980 (BNL)

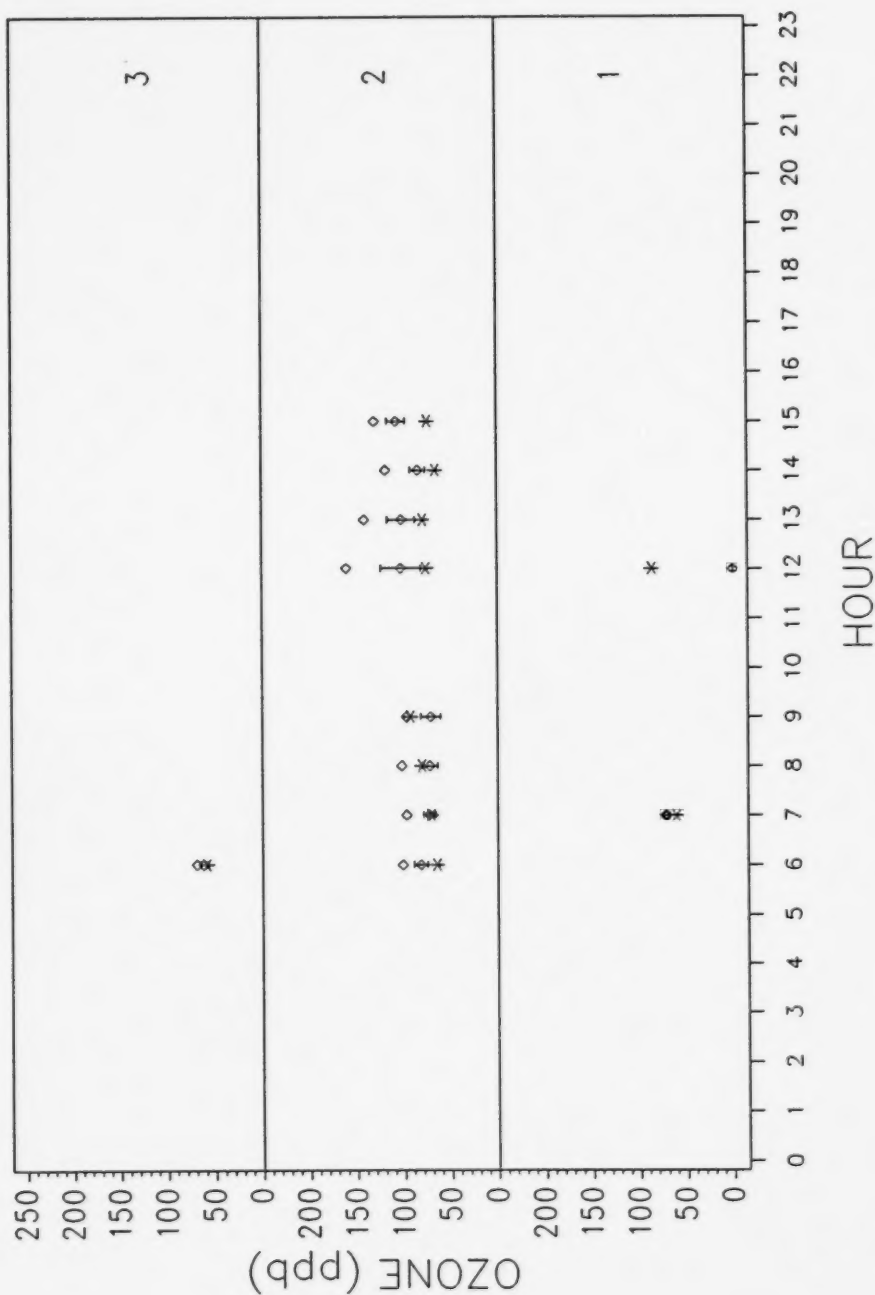


Figure 8.38. Time series of O₃ data from flight on July 19, 1980 in Baltimore, MD area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

AIRCRAFT - BALTIMORE AREA JULY 19, 1980 (WSU)

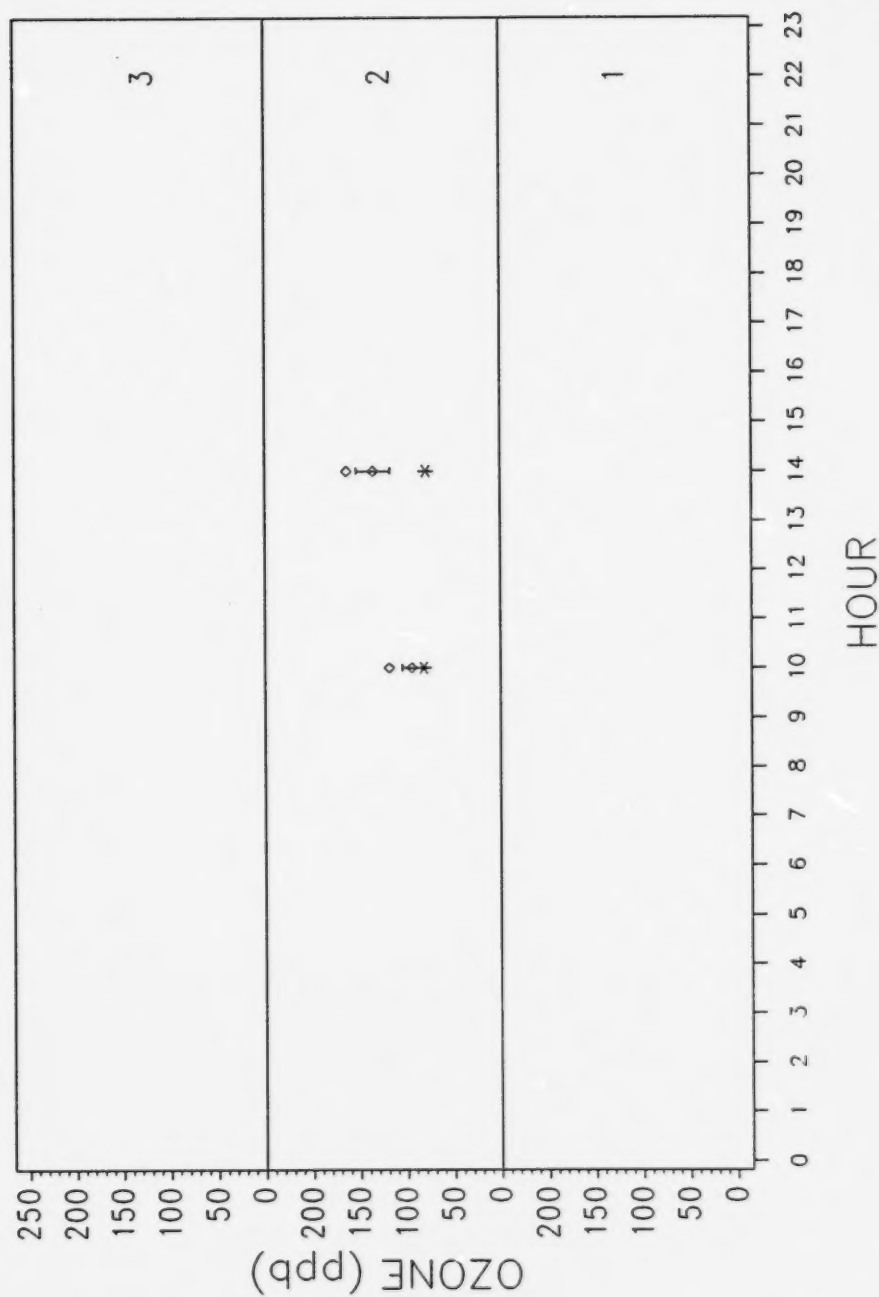
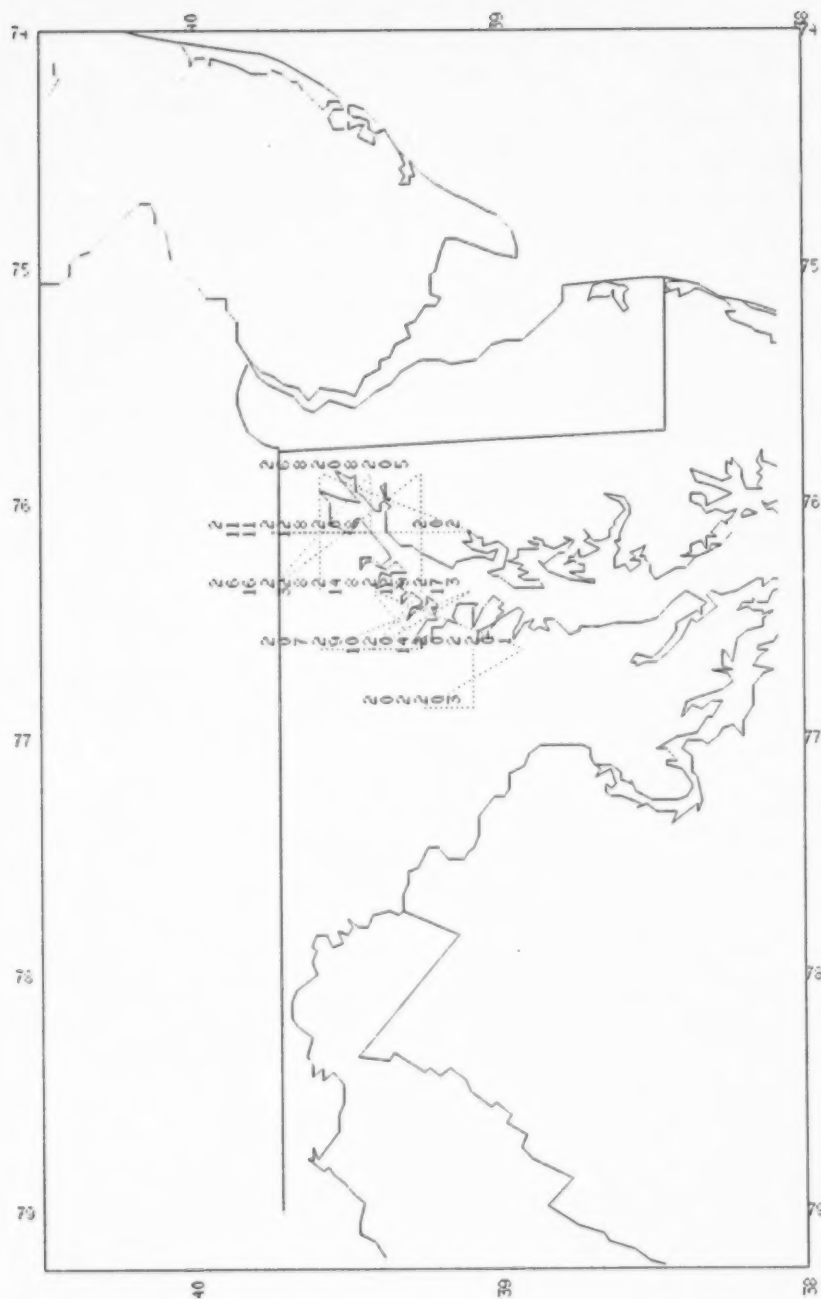


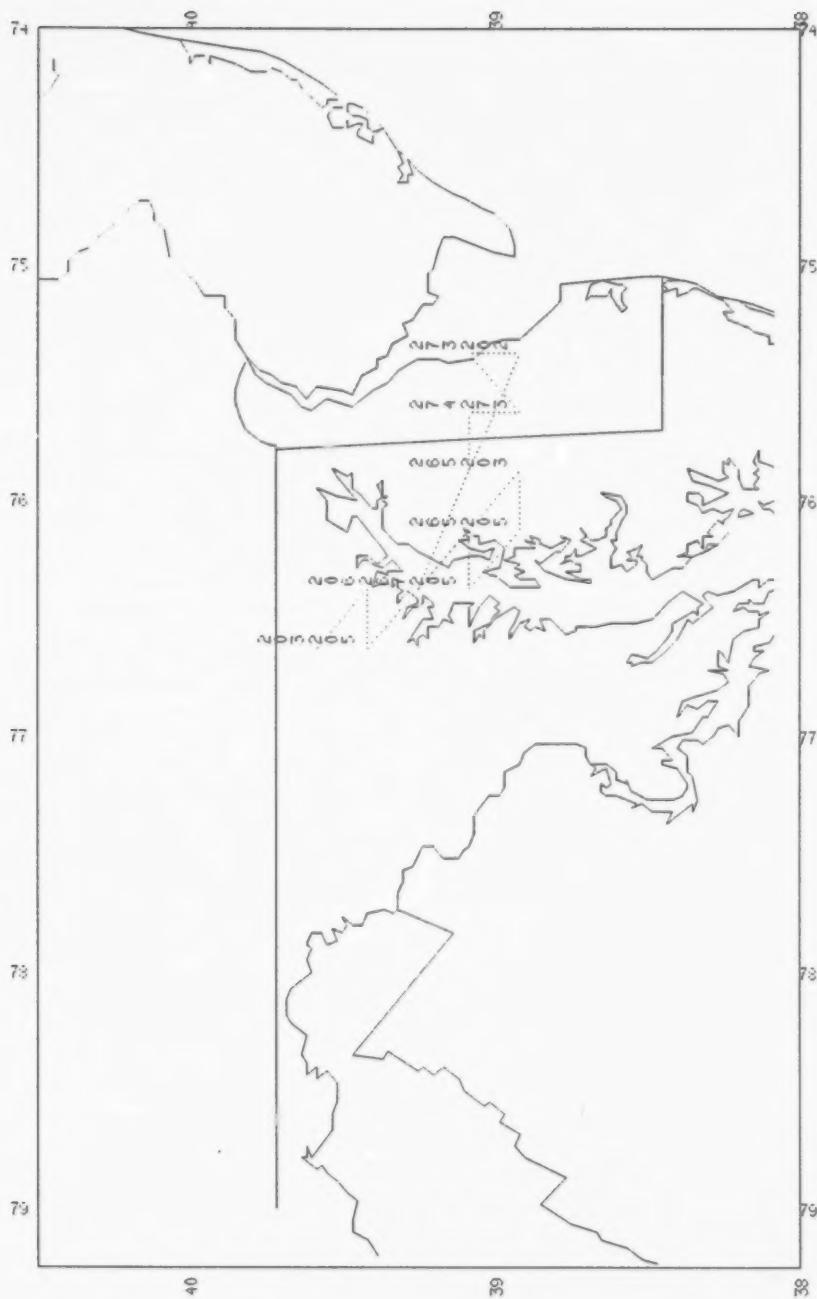
Figure 8.38 (cont.)



BALTIMORE (EAL) 7/19/80 (HES 6-9) MIX

WMECH extent - rows 1:15 cols 20:40

Figure 8.39. Geographical distribution of selected NO_x data from flight on July 19, 1980 in Baltimore, MD area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).



BALTIMORE (BAL) 7/19/80 (HRS 12-15) MIX

NINOM extent - rows 1:15 cols 20:40

Figure 8.39 (cont.)

AIRCRAFT - BALTIMORE AREA JULY 19, 1980 (BNL)

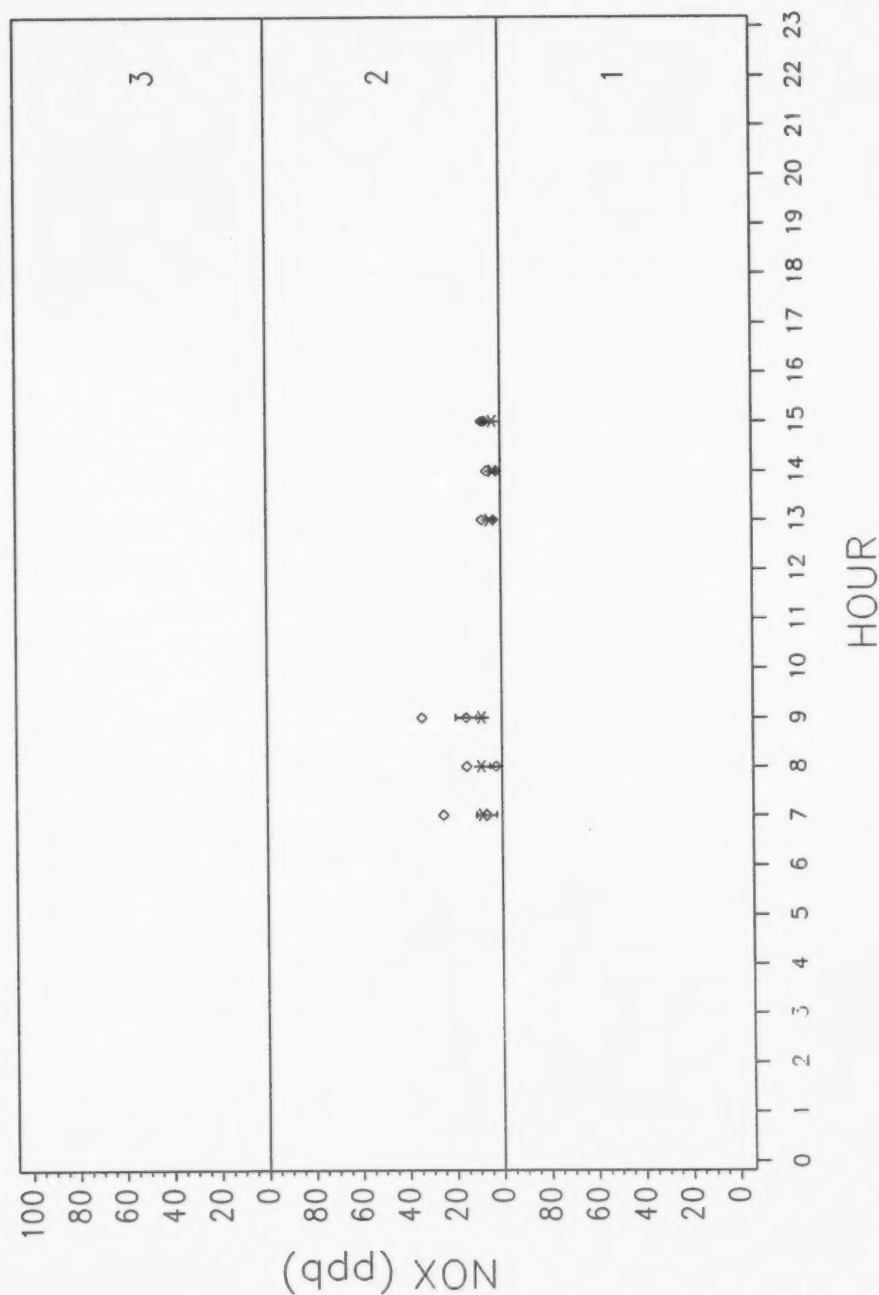


Figure 8.40. Time series of NO_x data from flight on July 19, 1980 in Baltimore, MD area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

AIRCRAFT - BALTIMORE AREA
JULY 19, 1980 (WSU)

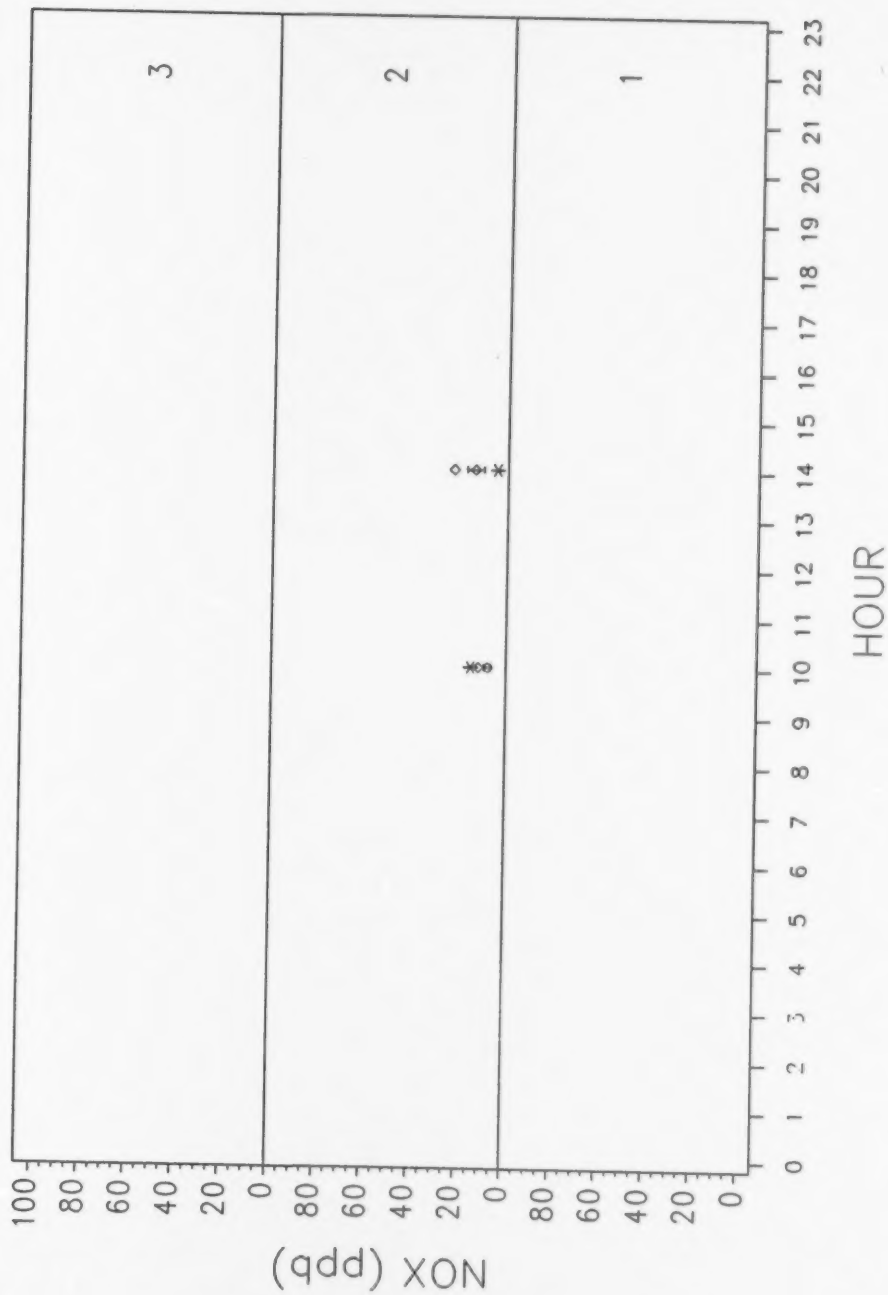


Figure 8.40 (cont.)

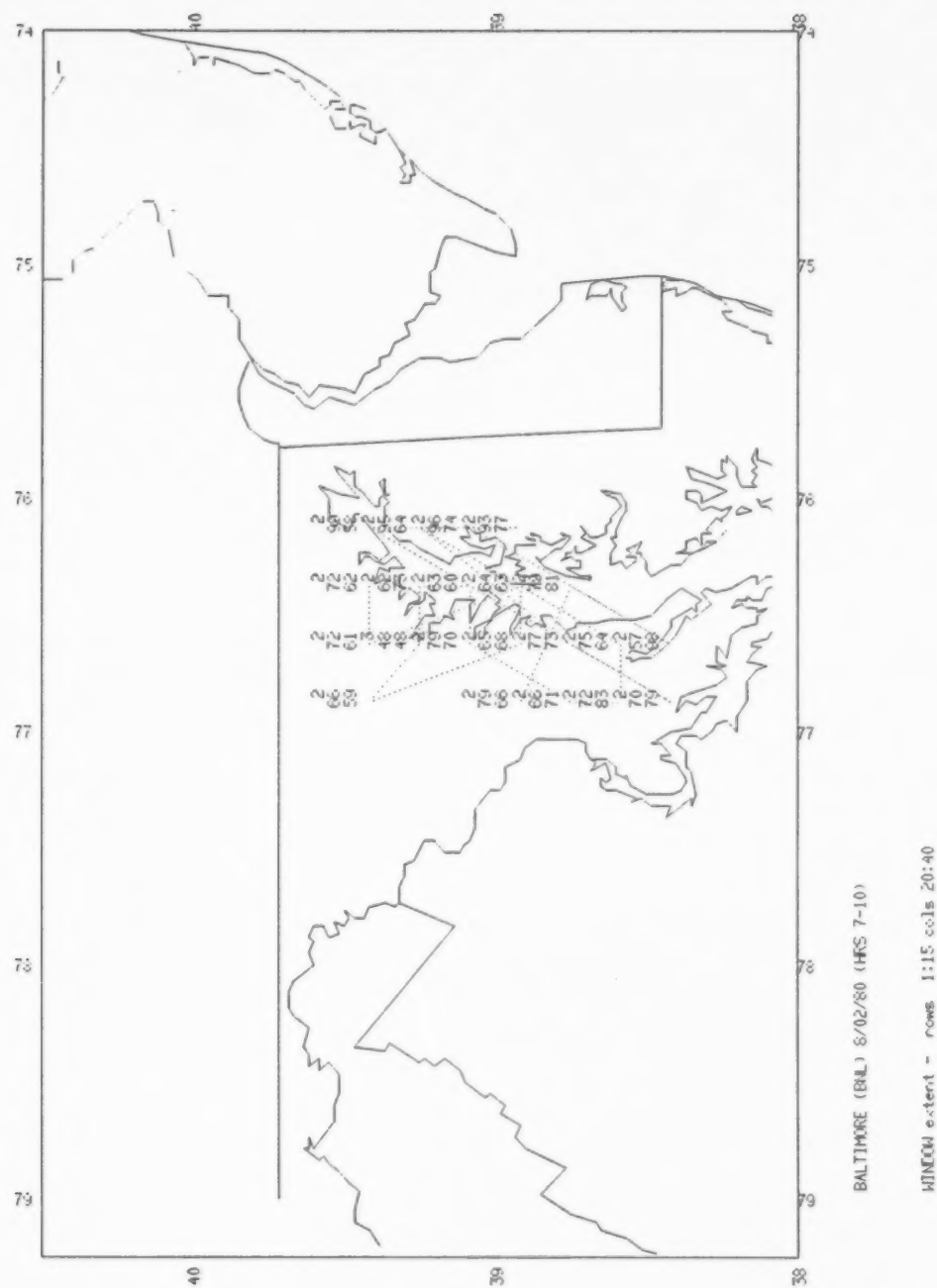
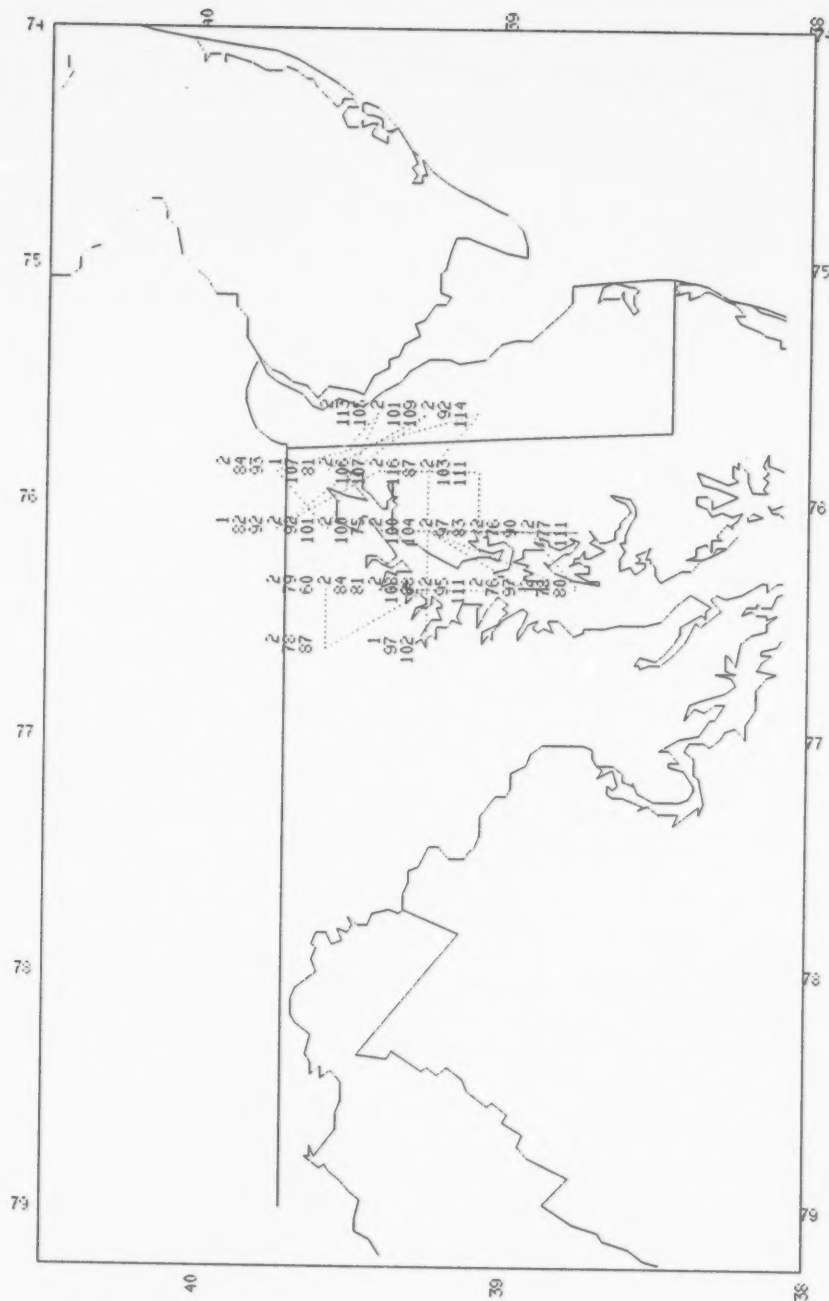


Figure 8.41. Geographical distribution of selected O_3 data from flight on Aug. 2, 1980 in Baltimore, MD area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).



BALTIMORE (BAL) 8/02/80 (HRS 15-18)

WINDOW extent - rows 1:15 cols 20:40

Figure 8.41 (cont.)

AIRCRAFT - BALTIMORE AREA AUGUST 2, 1980 (BNL)

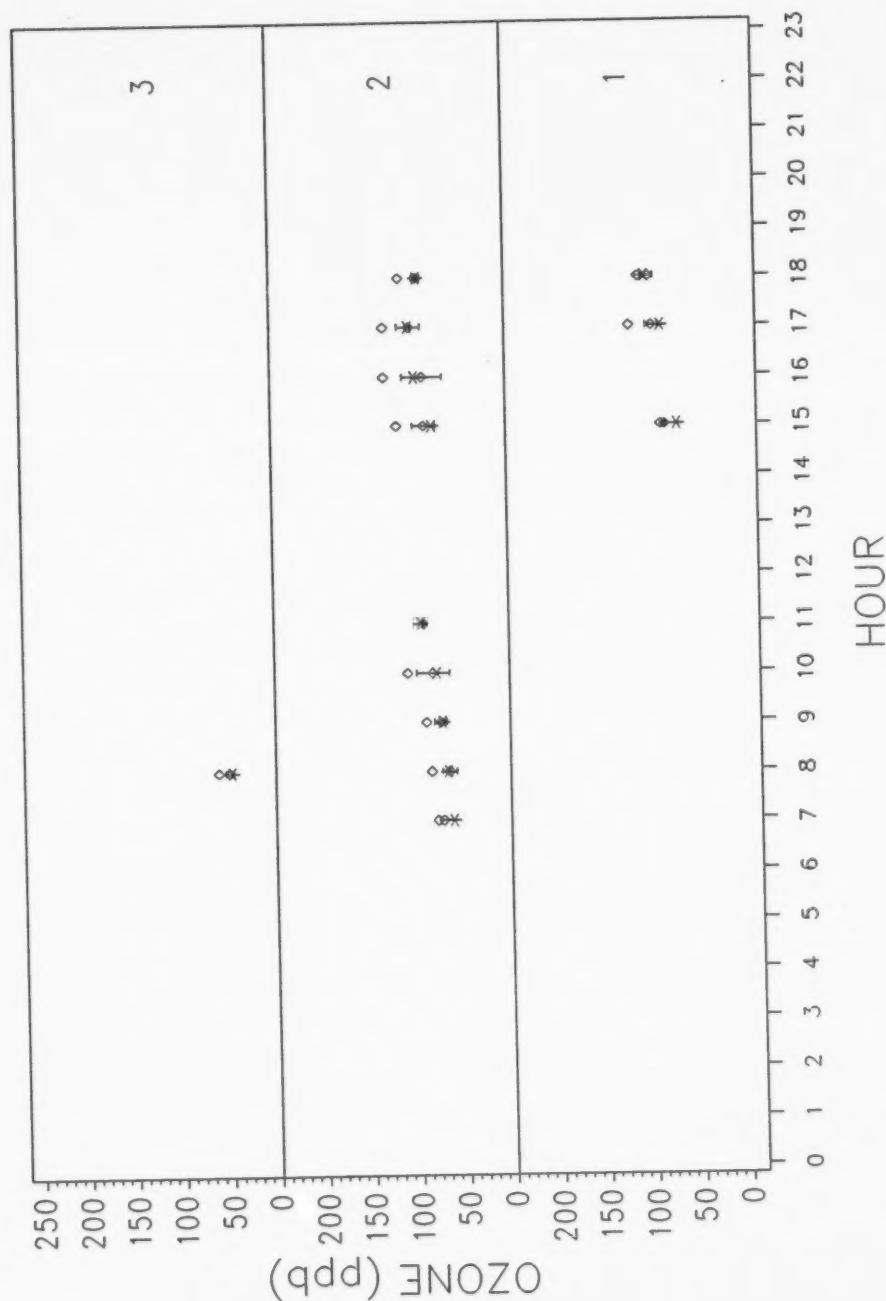


Figure 8.42. Time series of O₃ data from flight on Aug. 2, 1980 in Baltimore, MD area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

AIRCRAFT - BALTIMORE AREA
AUGUST 2, 1980 (WSU)

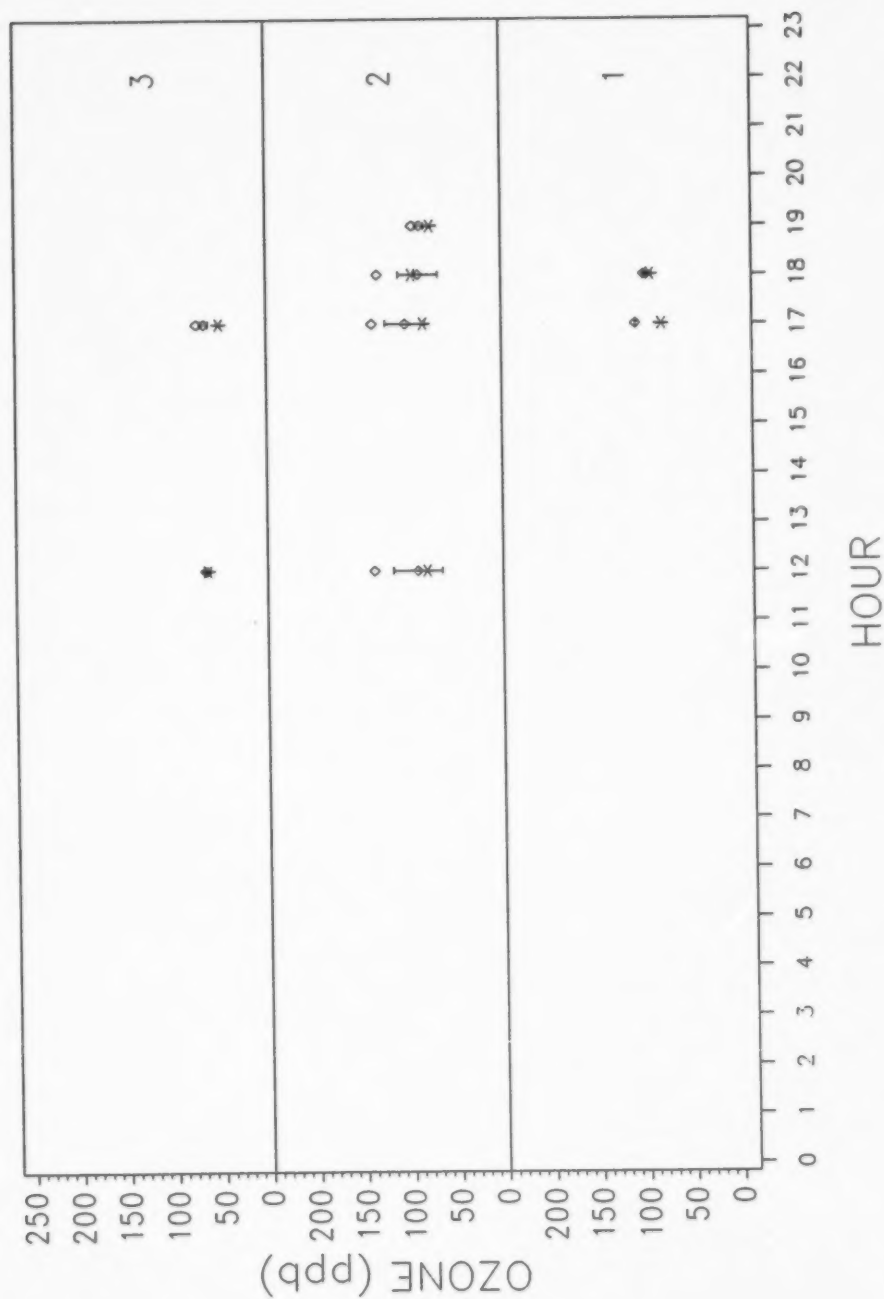


Figure 8.42 (cont.)

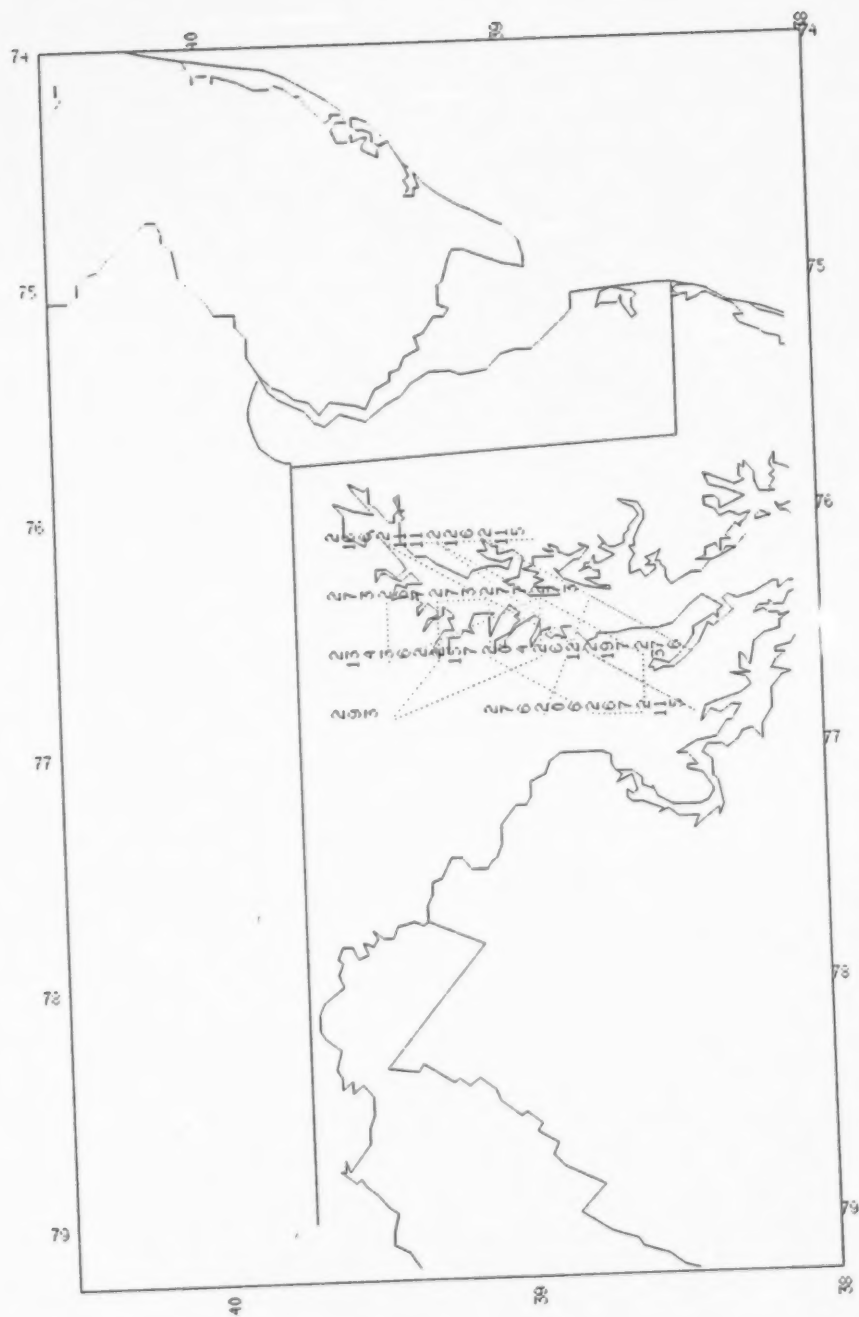
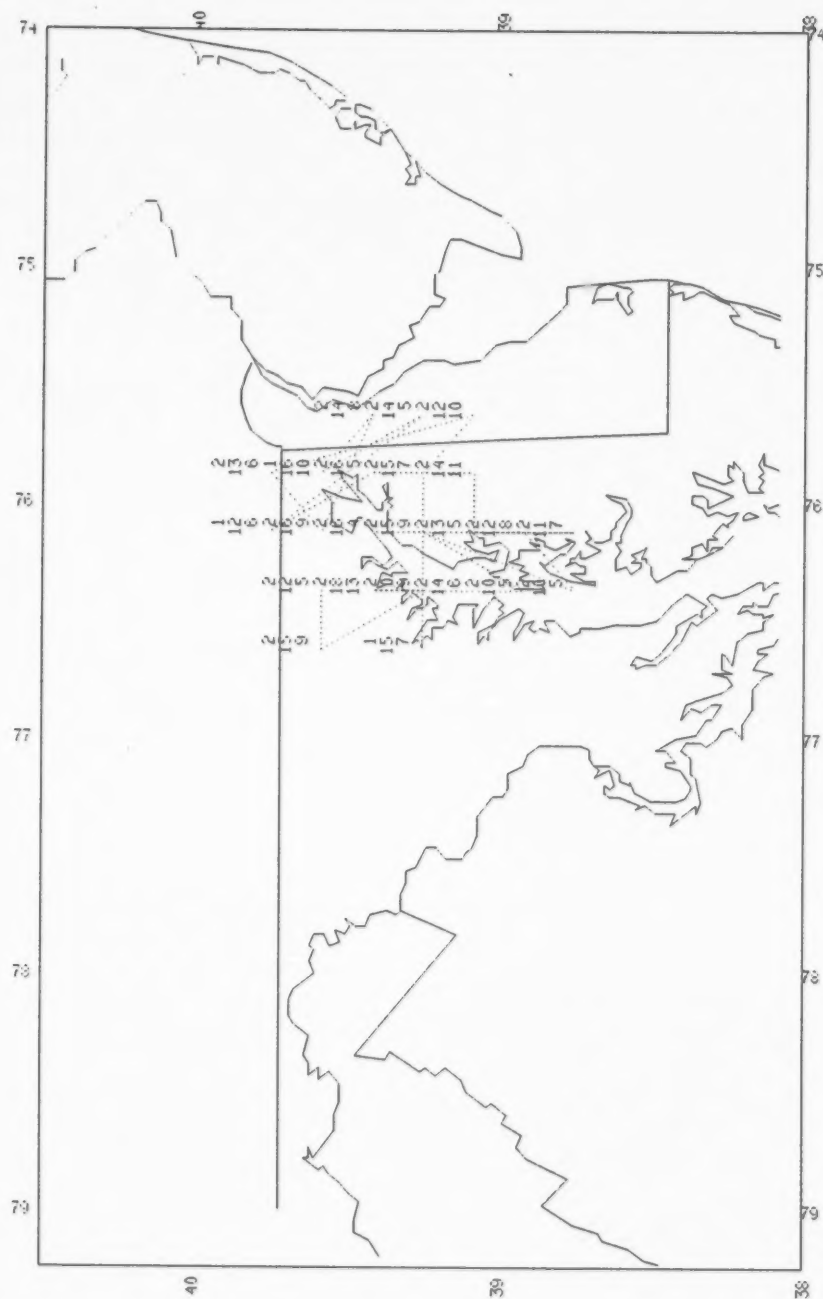


Figure 8.43. Geographical distribution of selected NO_x data from flight on Aug. 2, 1980 in Baltimore, MD area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).



BALTIMORE (BAL) S/02/80 (HRS 15-18) NXX

WIND extent - rows 1:15 cols 20:40

Figure 8.43 (cont.)

AIRCRAFT - BALTIMORE AREA AUGUST 2, 1980 (BNL)

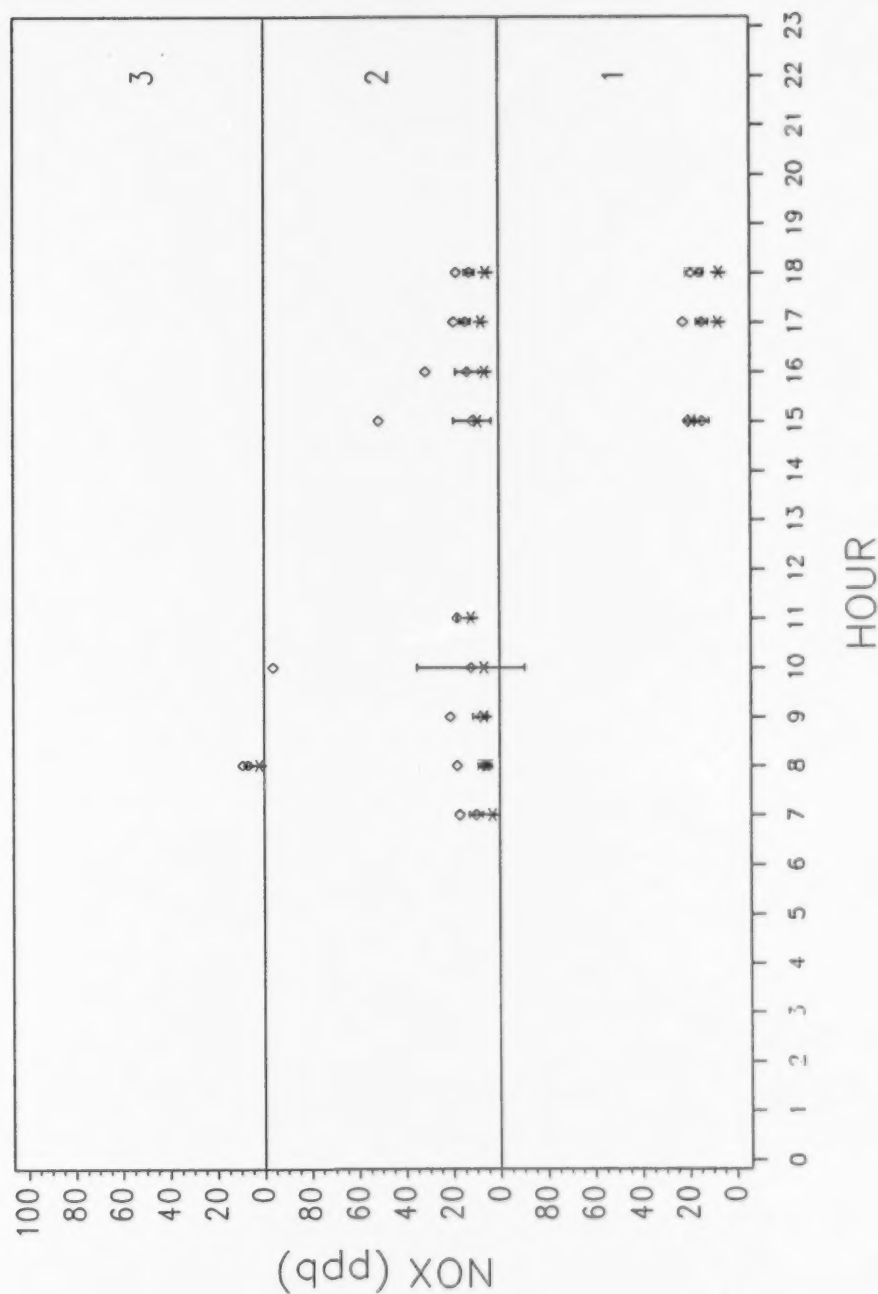


Figure 8.44. Time series of NO_x data from flight on Aug. 2, 1980 in Baltimore, MD area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

AIRCRAFT - BALTIMORE AREA
AUGUST 2, 1980 (WSU)

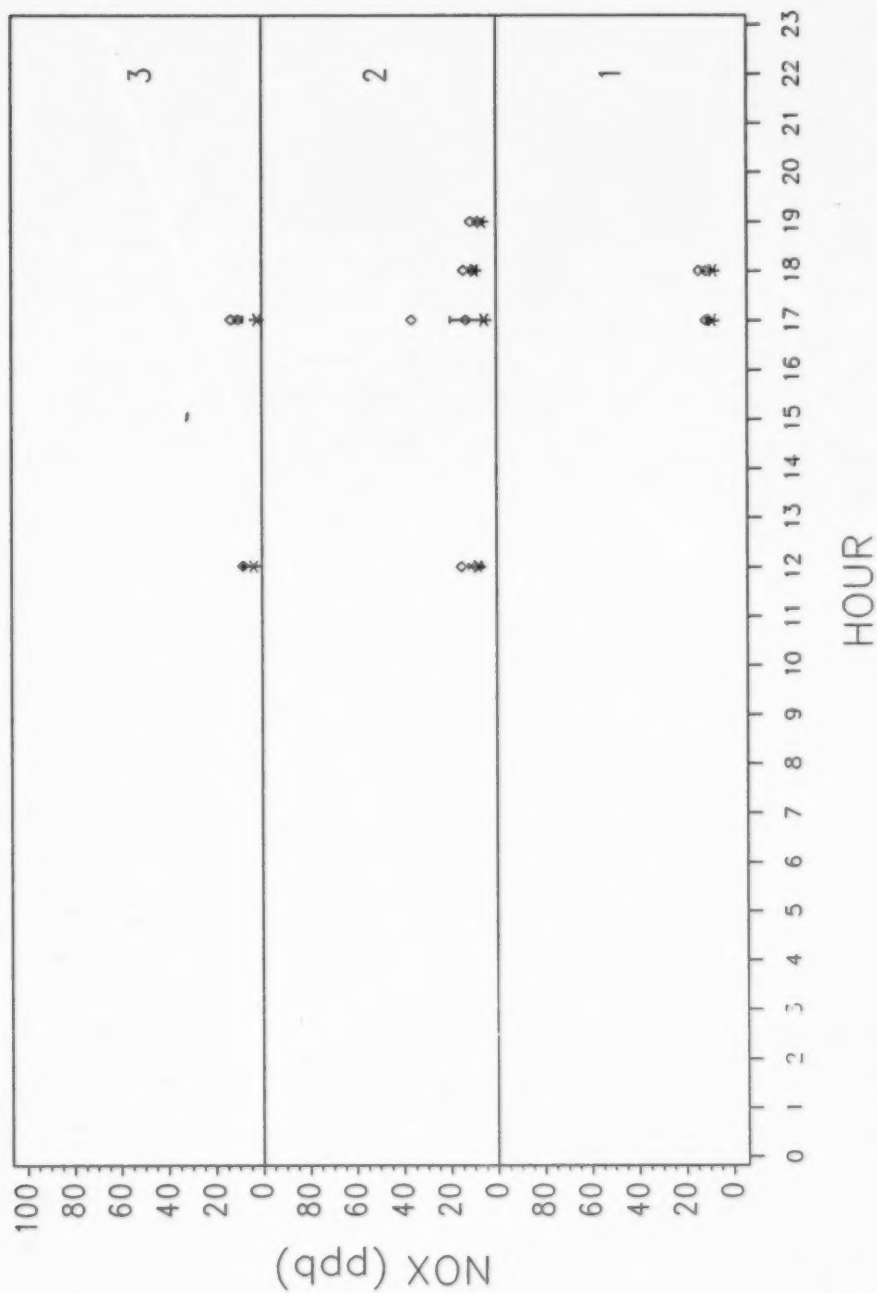


Figure 8.44 (cont.)

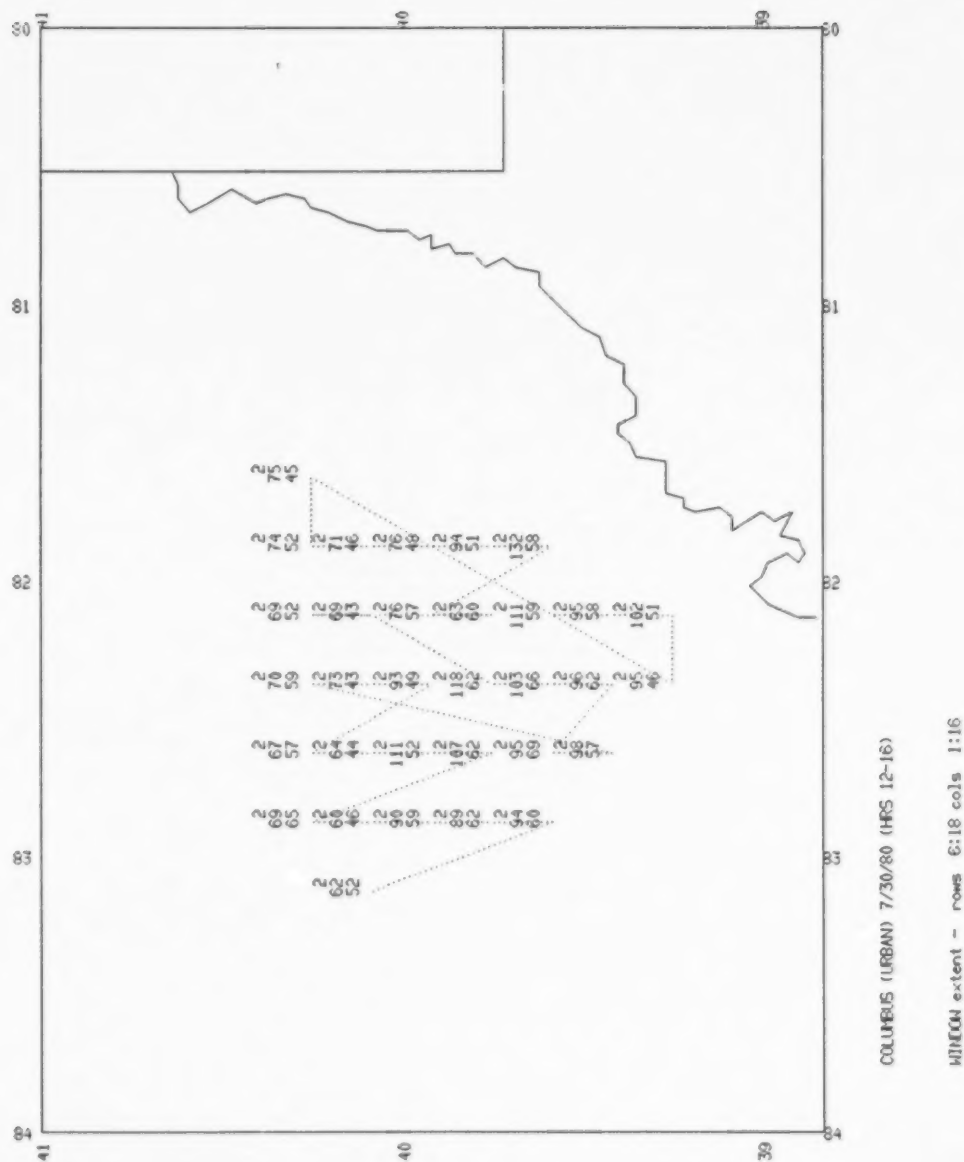


Figure 8.45. Geographical distribution of selected O_3 data from flight on July 30, 1980 in Columbus, OH area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - COLUMBUS (URBAN)
JULY 30, 1980 (AV)
LAYER 2

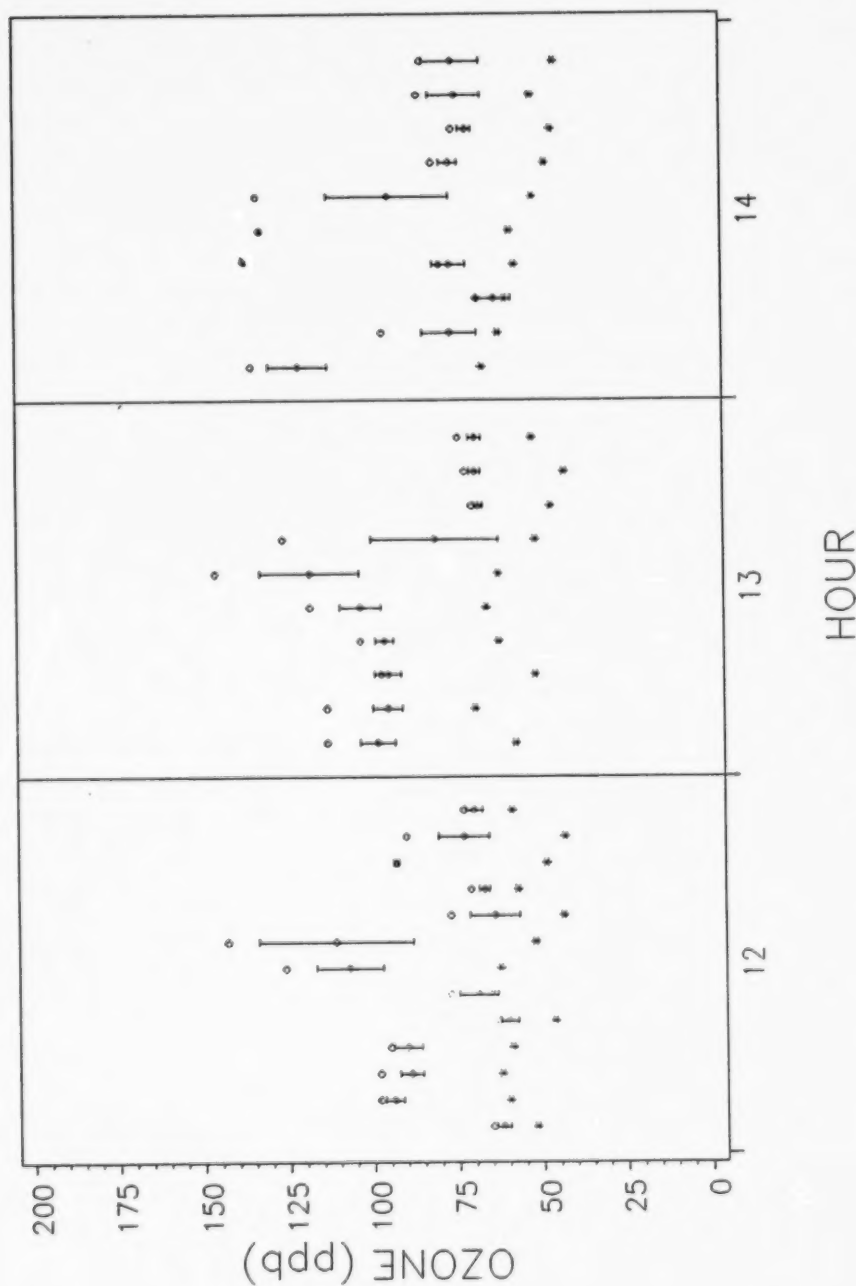


Figure 8.46. Time series of O_3 data from flight on July 30, 1980 in Columbus, OH area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

AIRCRAFT - COLUMBUS (URBAN)
JULY 30, 1980 (AV)
LAYER 2

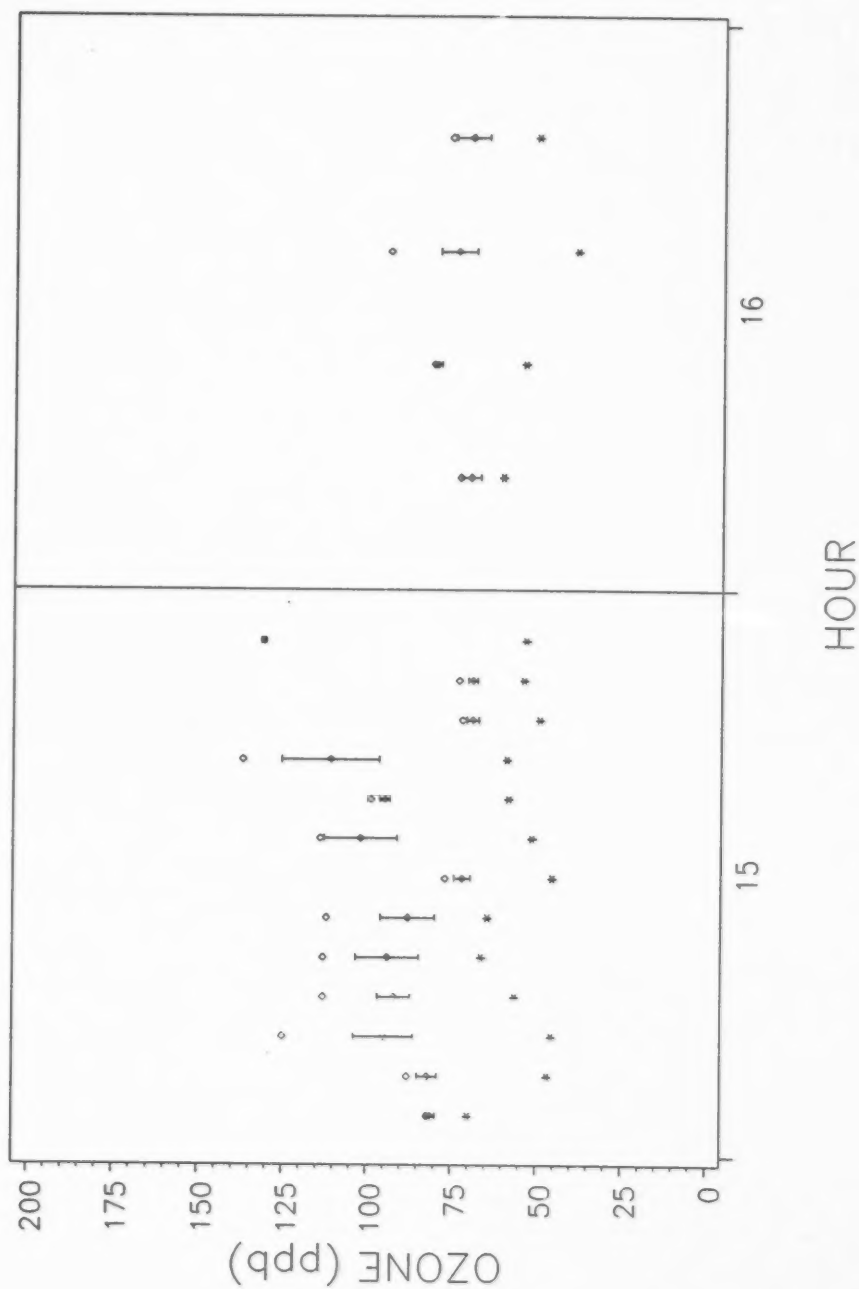


Figure 8.46 (cont.)

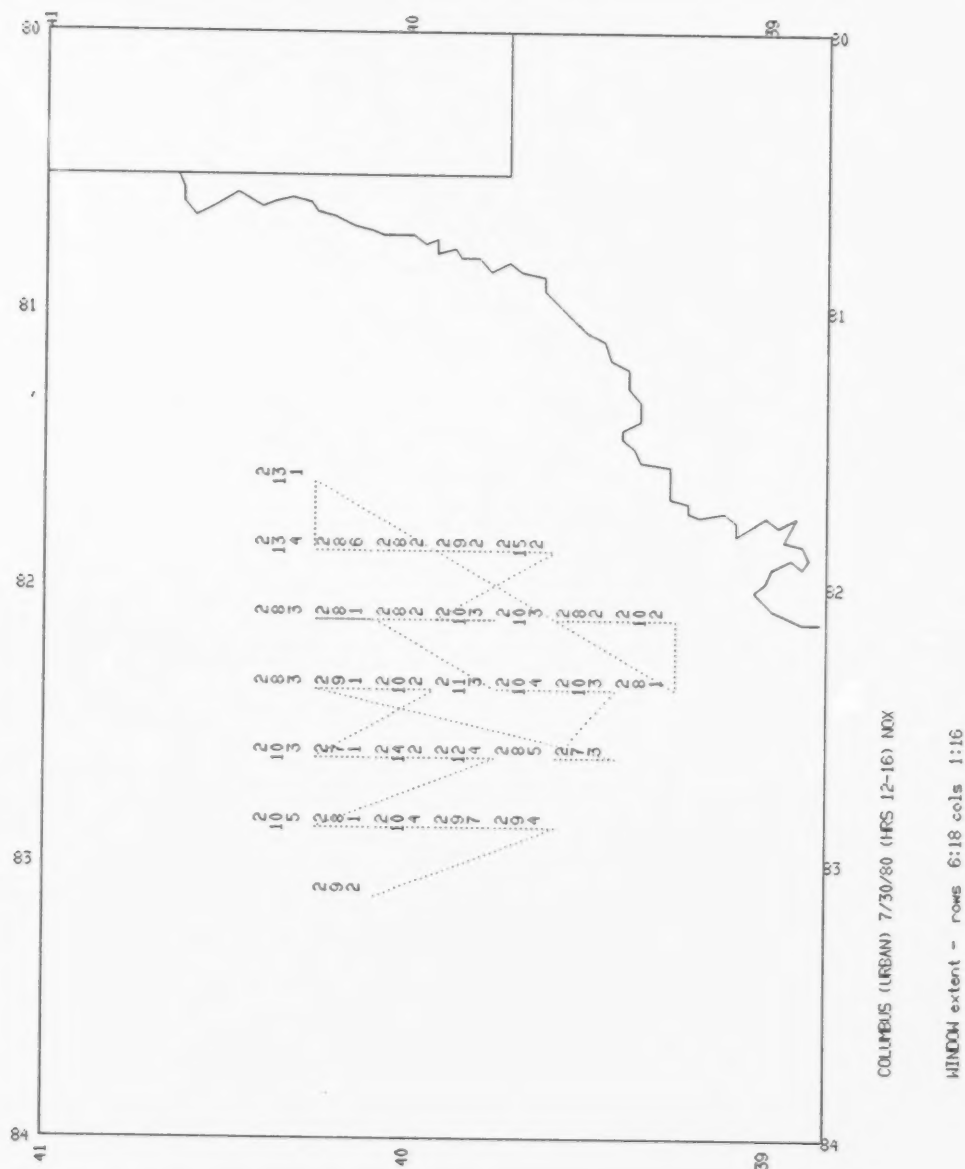


Figure 8.47. Geographical distribution of selected NO_x data from flight on July 30, 1980 in Columbus, OH area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - COLUMBUS (URBAN)
JULY 30, 1980 (AV)
LAYER 2

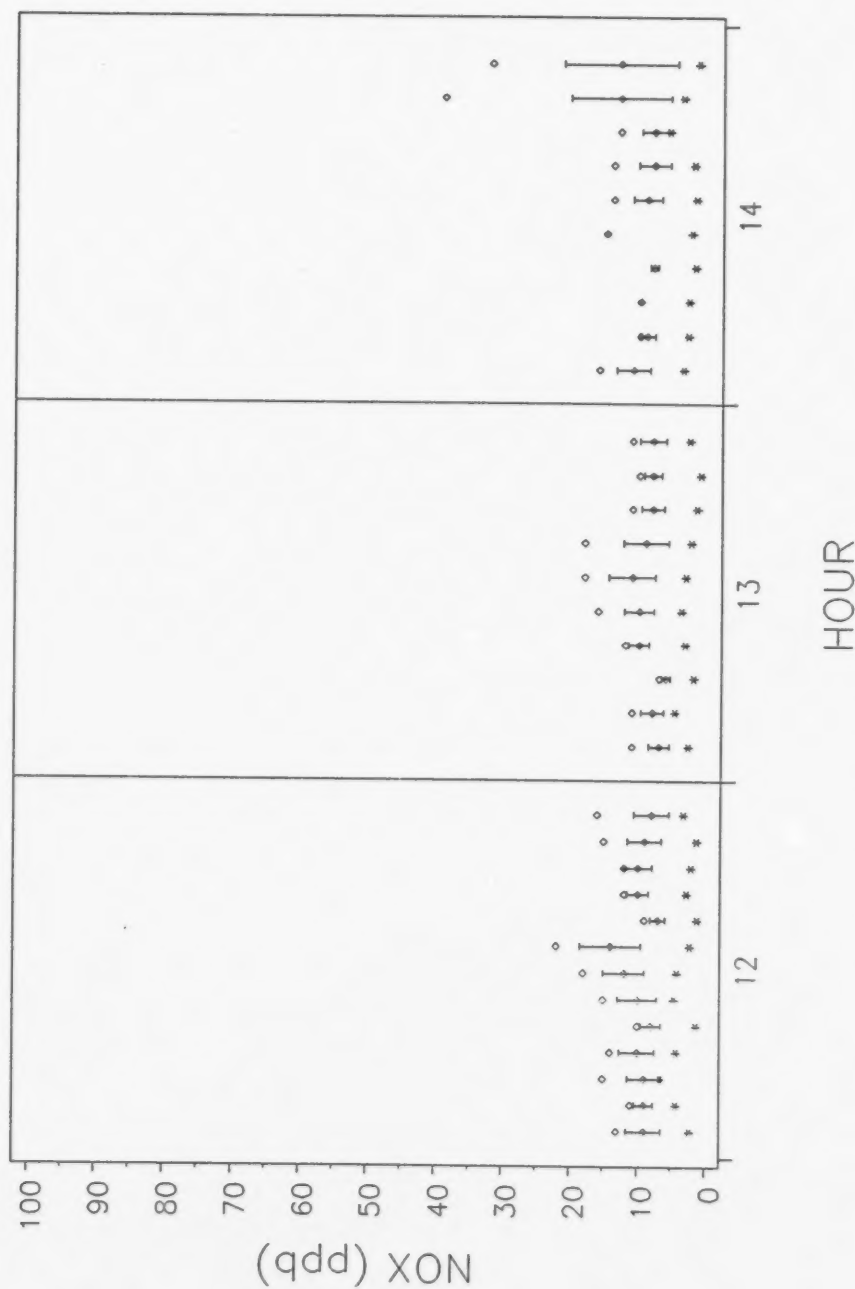


Figure 8.48. Time series of NO_x data from flight on July 30, 1980 in Columbus, OH area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

AIRCRAFT - COLUMBUS (URBAN)
JULY 30, 1980 (AV)
LAYER 2

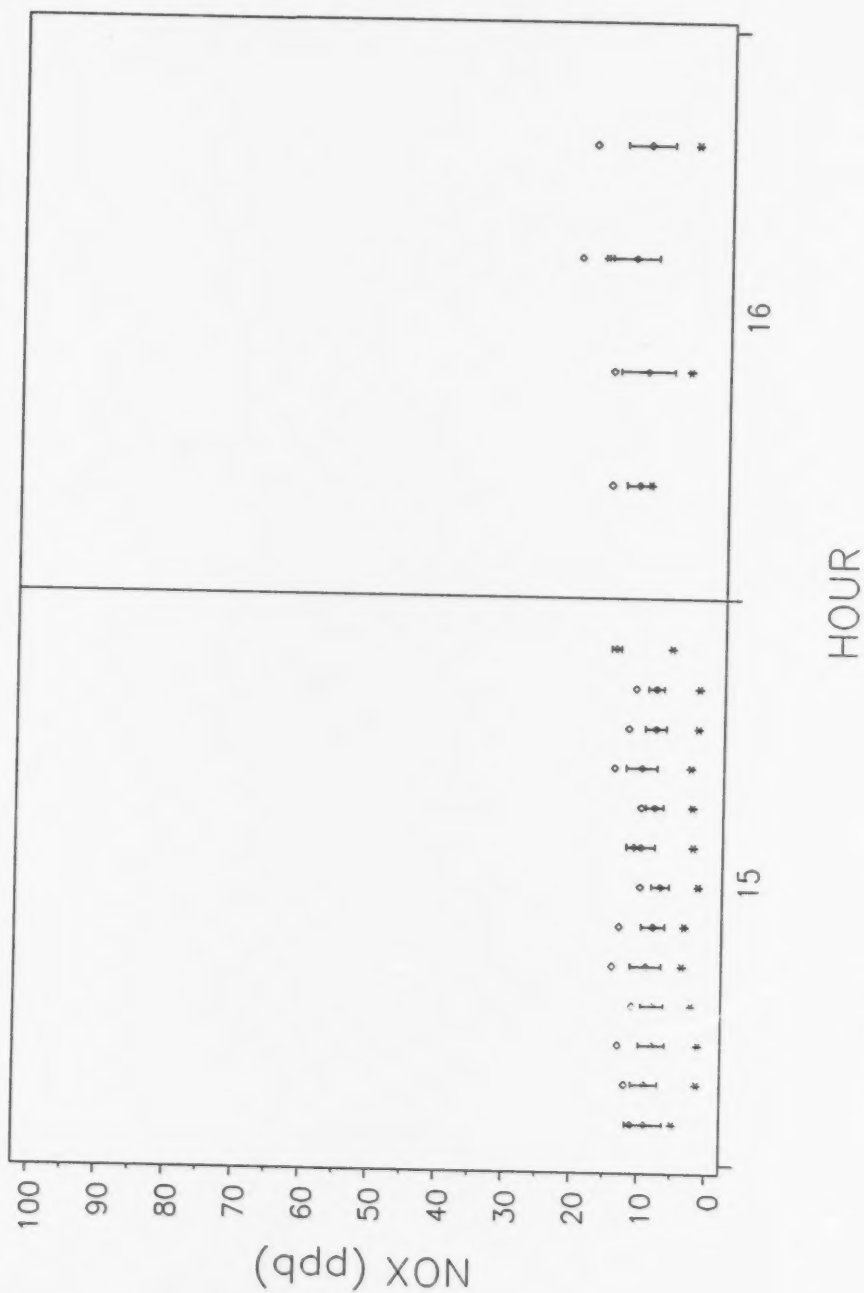


Figure 8.48 (cont.)

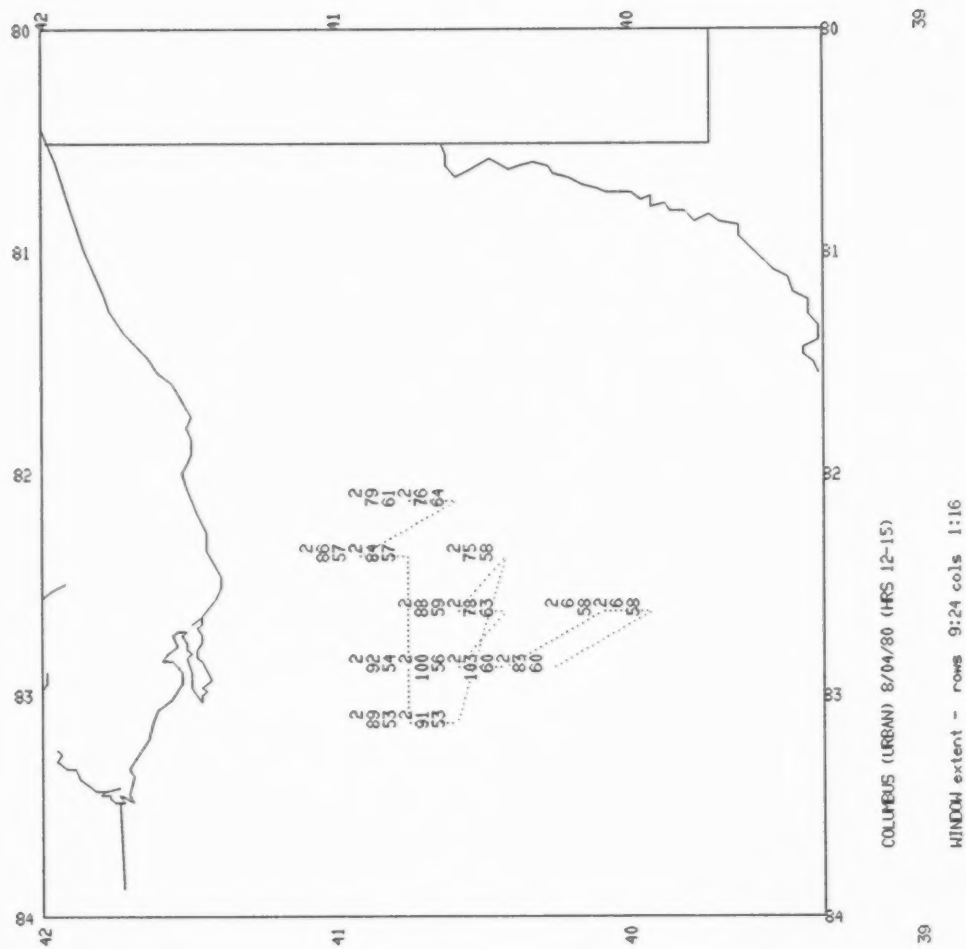


Figure 8.49. Geographical distribution of selected O₃ data from flight on Aug. 4, 1980 in Columbus, OH area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - COLUMBUS (URBAN)
AUGUST 4, 1980 (AV)
LAYER 2

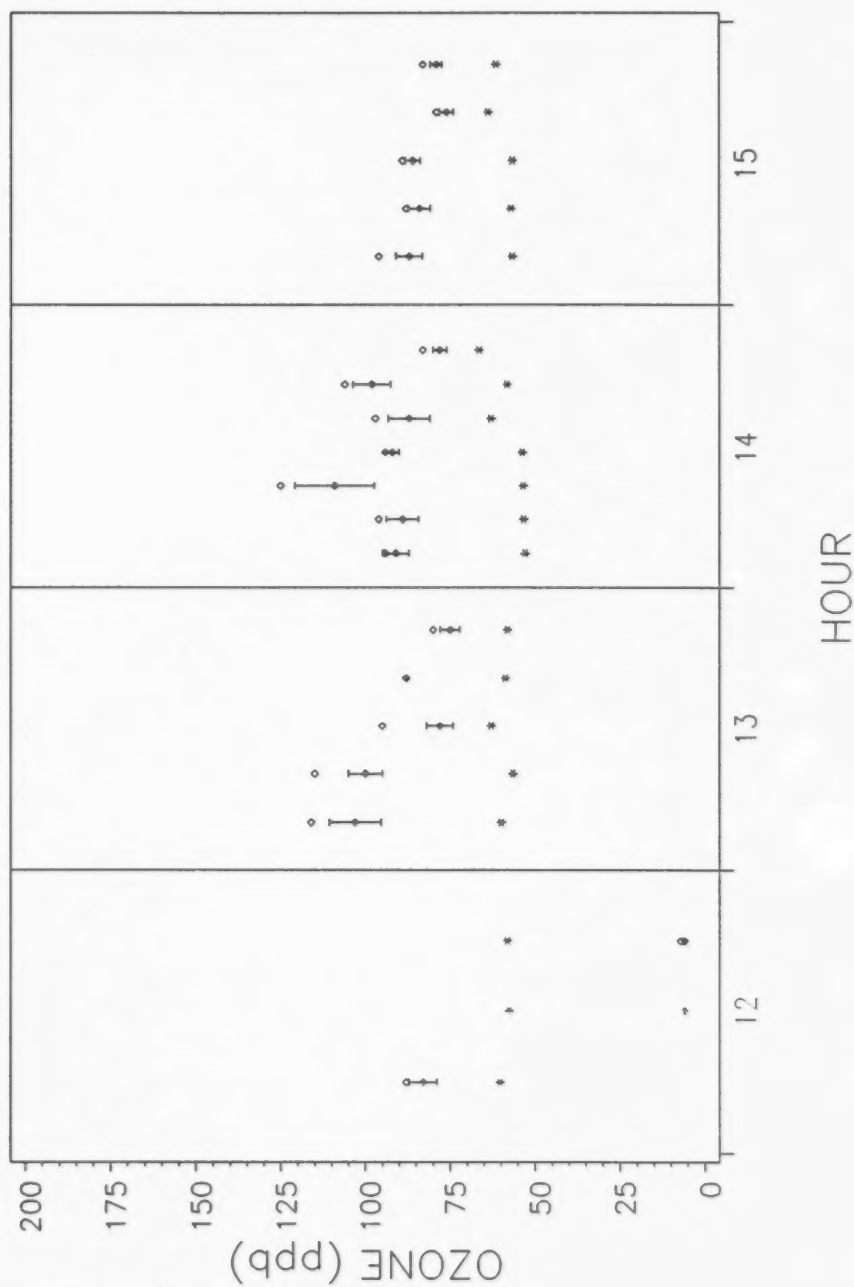


Figure 8.50. Time series of O₃ data from flight on Aug. 4, 1980 in Columbus, OH area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

AIRCRAFT - COLUMBUS (URBAN)
AUGUST 4, 1980 (AV)
LAYER 2

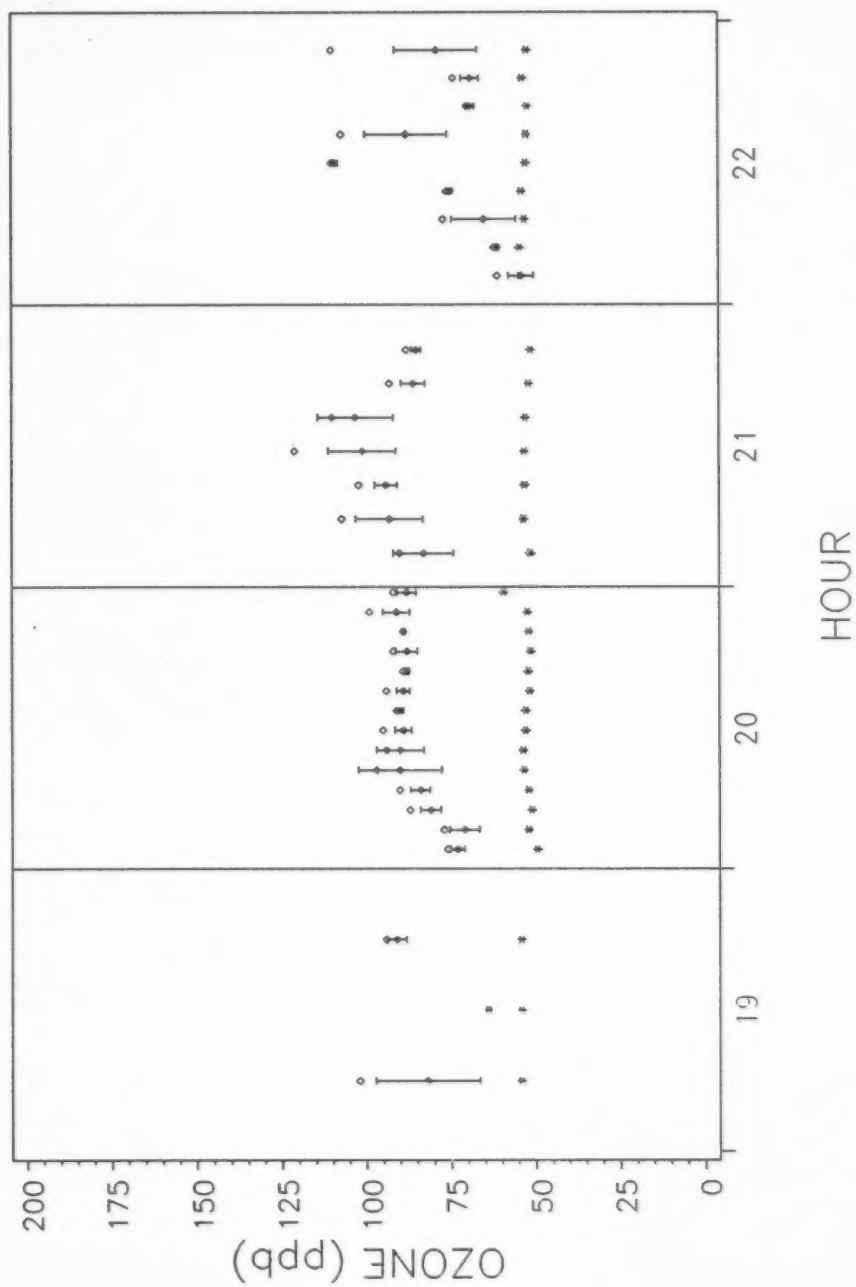


Figure 8.50 (cont.)

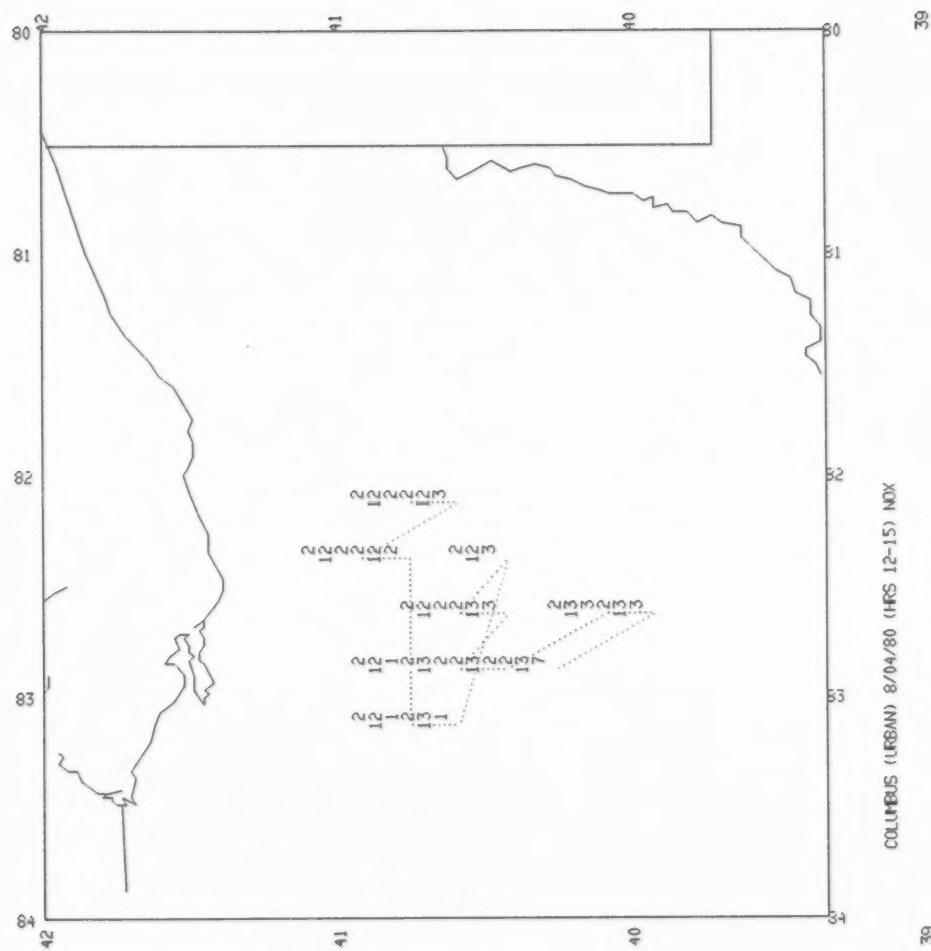


Figure 8.51. Geographical distribution of selected NO_x data from flight on Aug. 4, 1980 in Columbus, OH area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

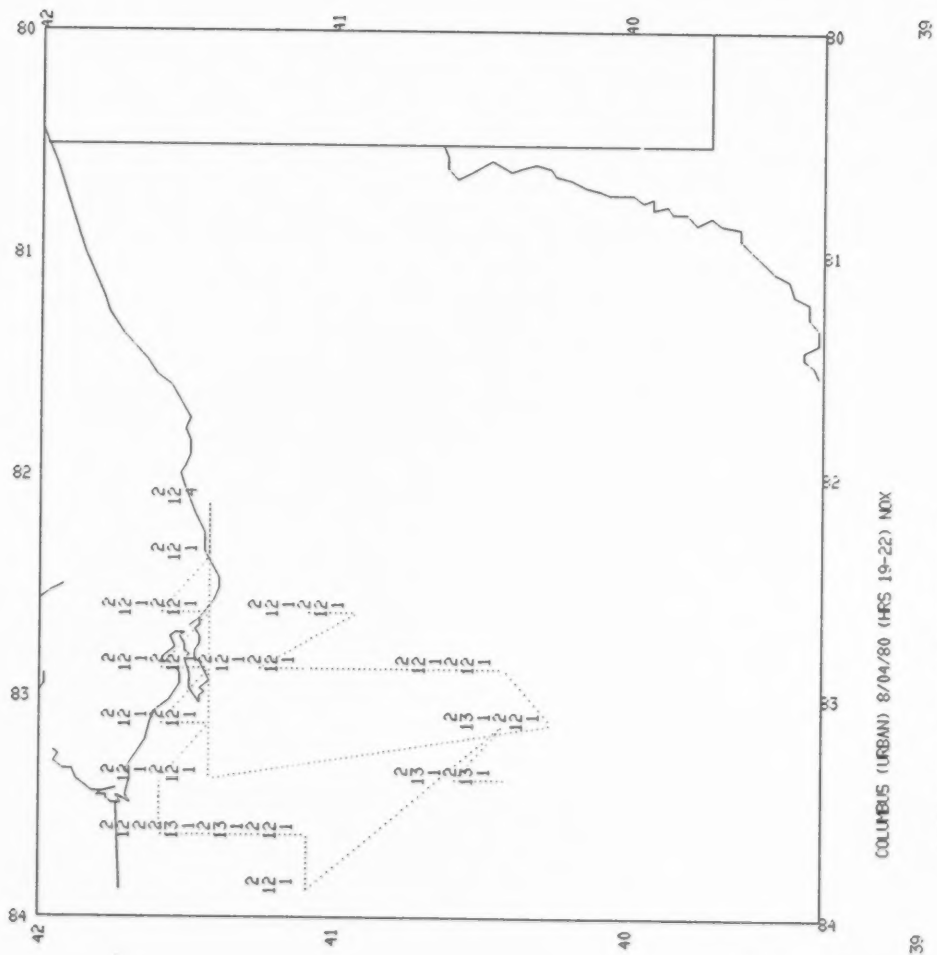


Figure 8.51 (cont.)

AIRCRAFT - COLUMBUS (URBAN)
AUGUST 4, 1980 (AV)
LAYER 2

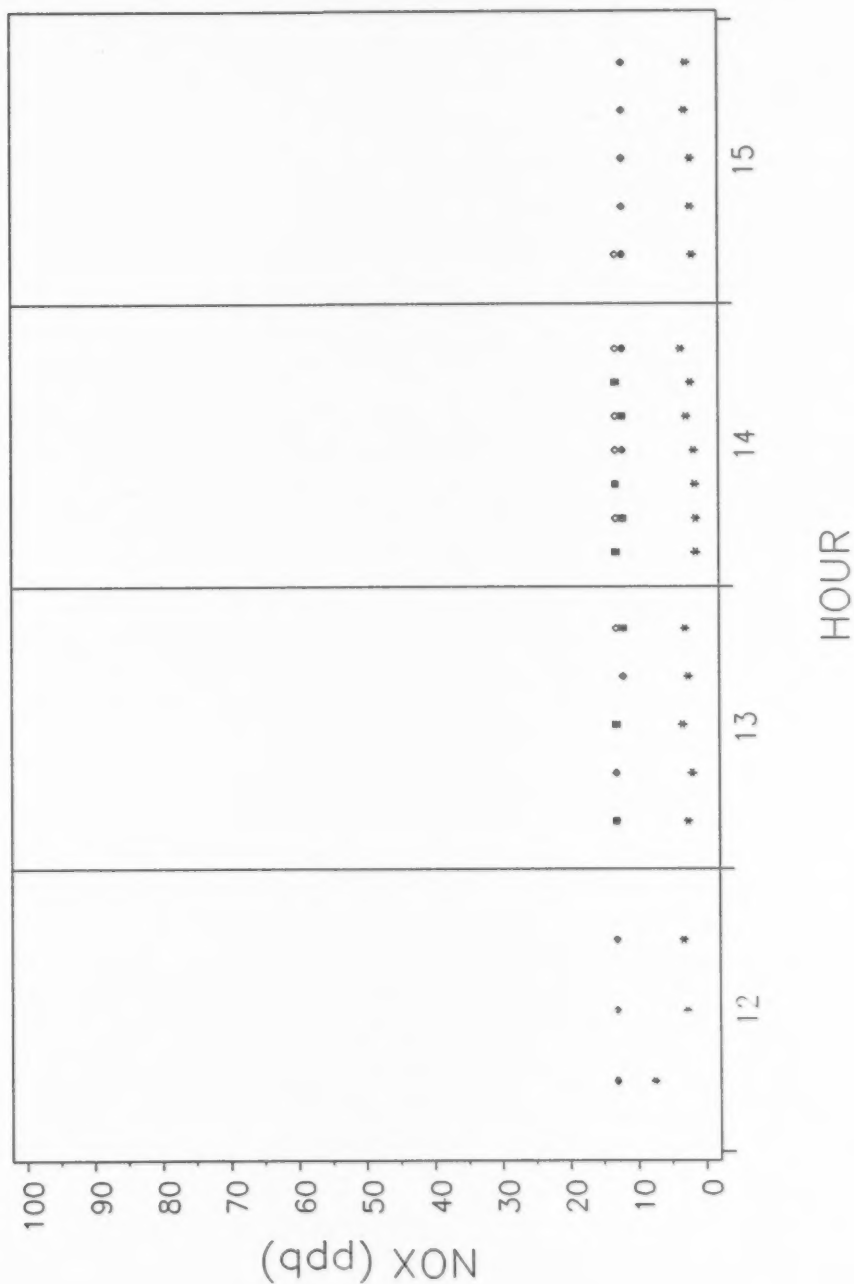


Figure 8.52. Time series of NO_x data from flight on Aug. 4, 1980 in Columbus, OH area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

AIRCRAFT - COLUMBUS (URBAN)
AUGUST 4, 1980 (AV)
LAYER 2

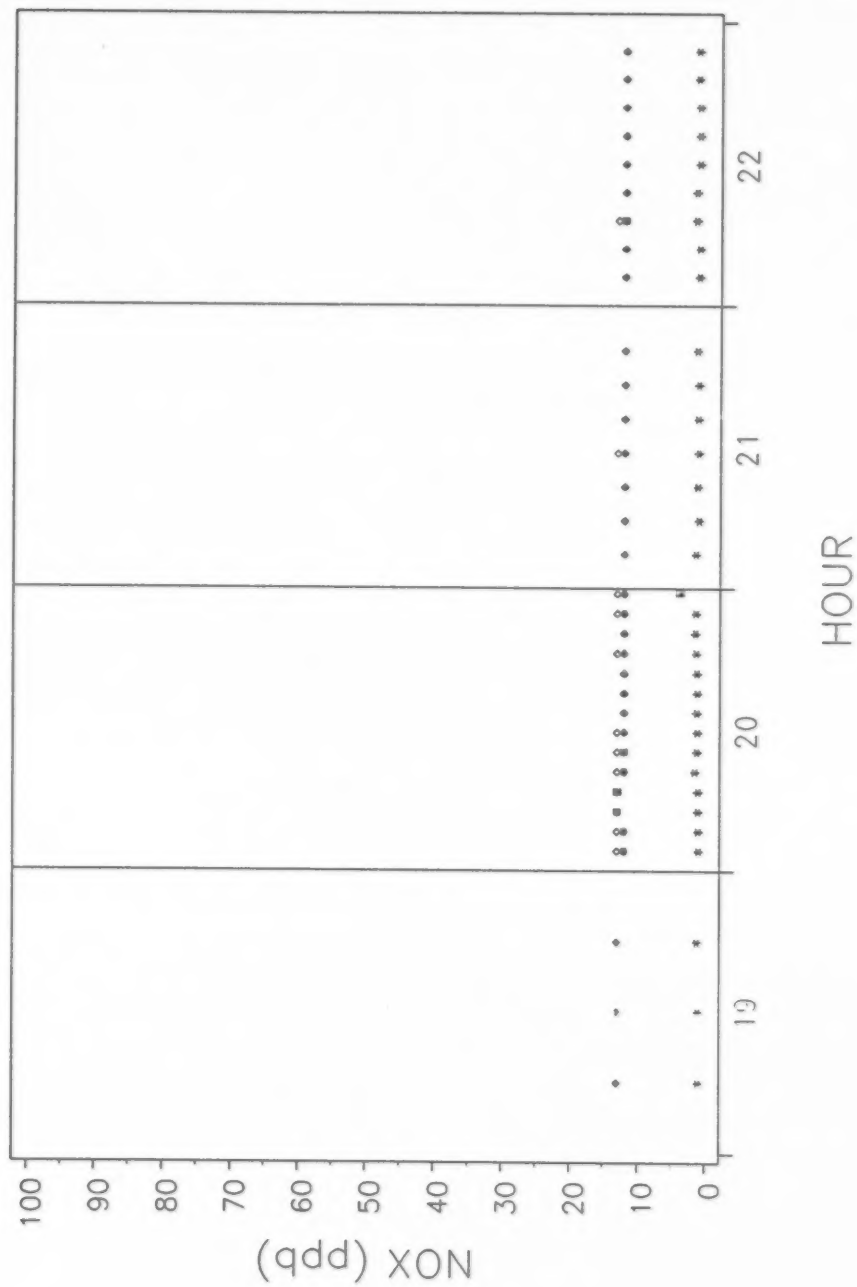


Figure 8.52 (cont.)

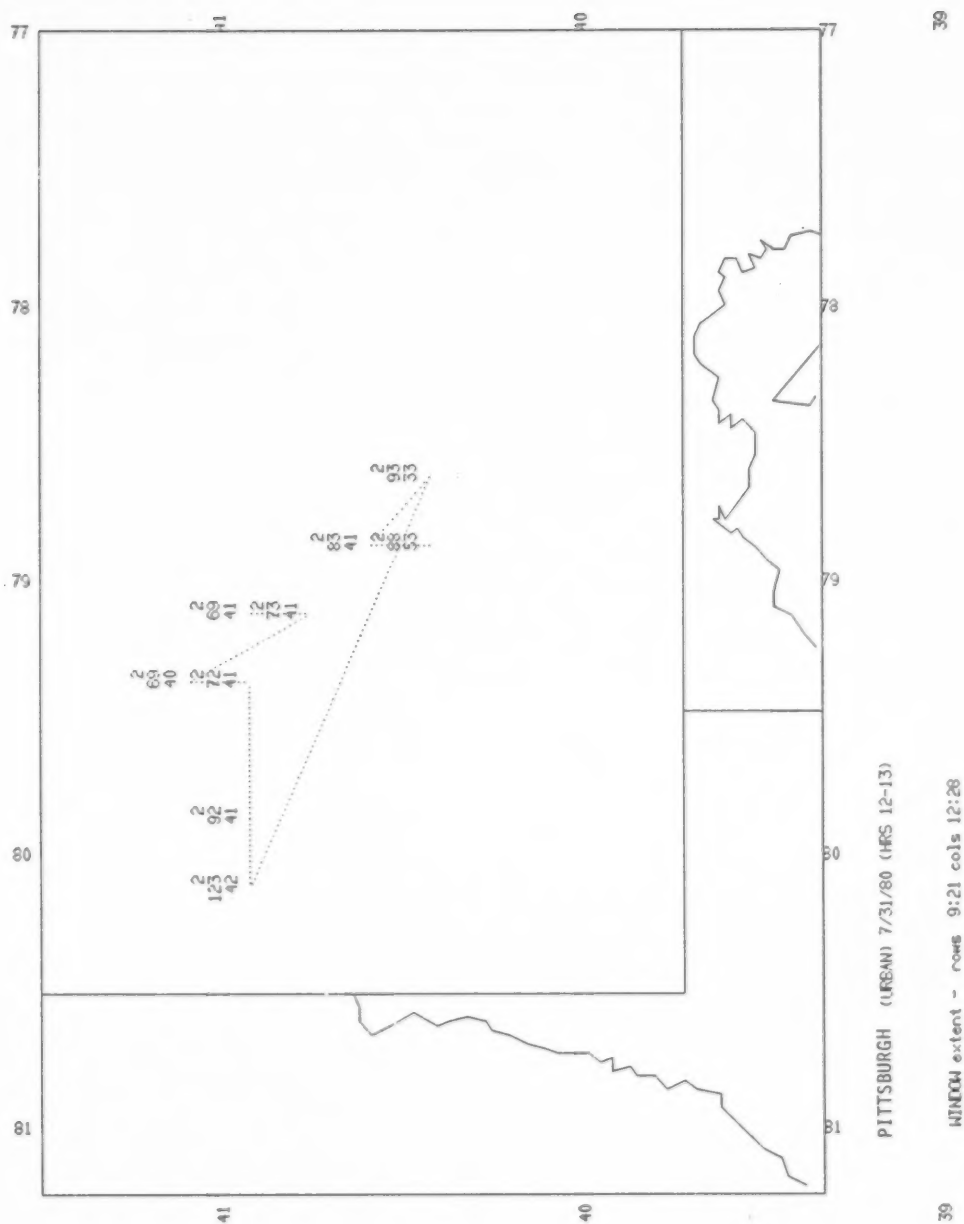


Figure 8.53. Geographical distribution of selected O_3 data from flight on July 31, 1980 in Pittsburgh, PA area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - PITTSBURGH (URBAN)
JULY 31, 1980 (AV)
LAYER 2

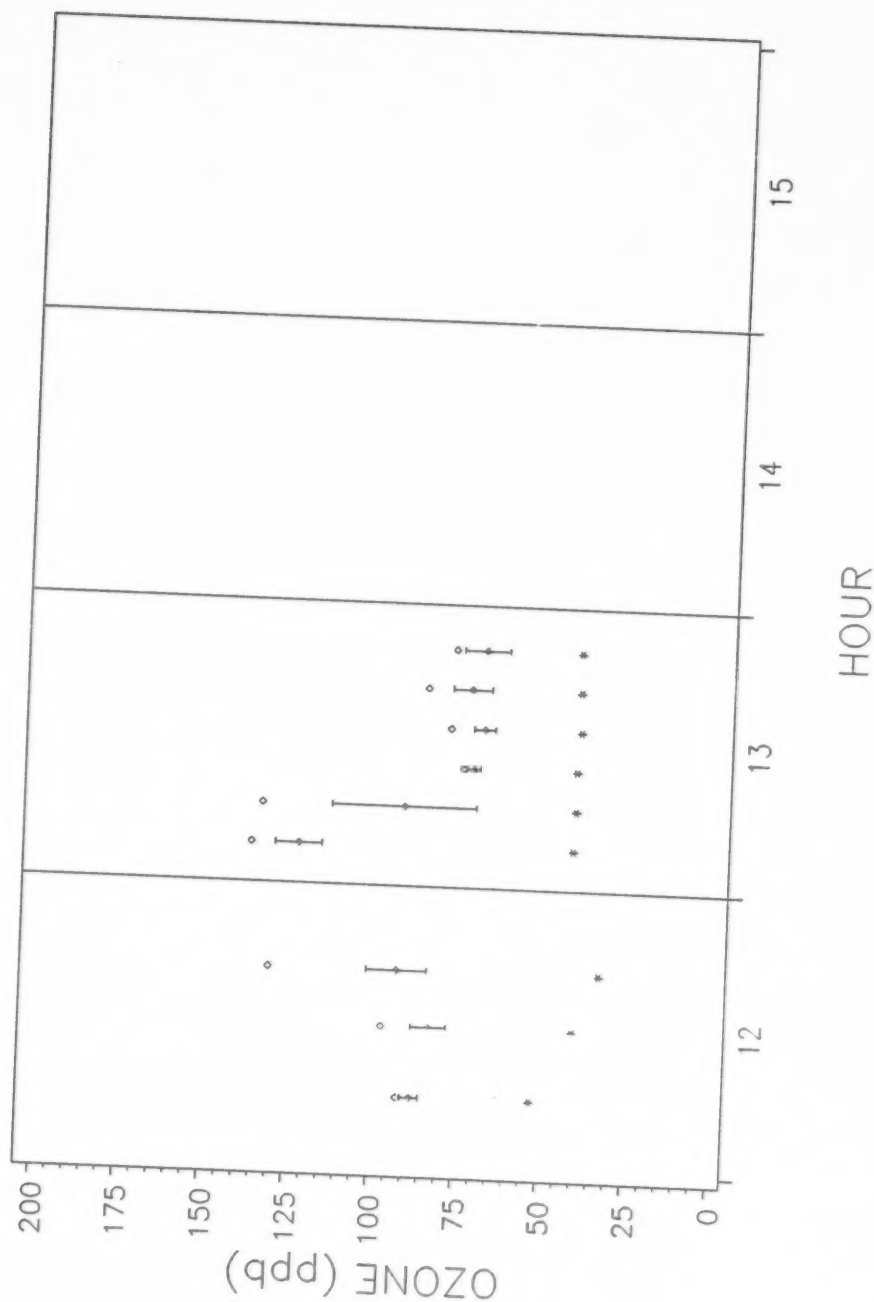
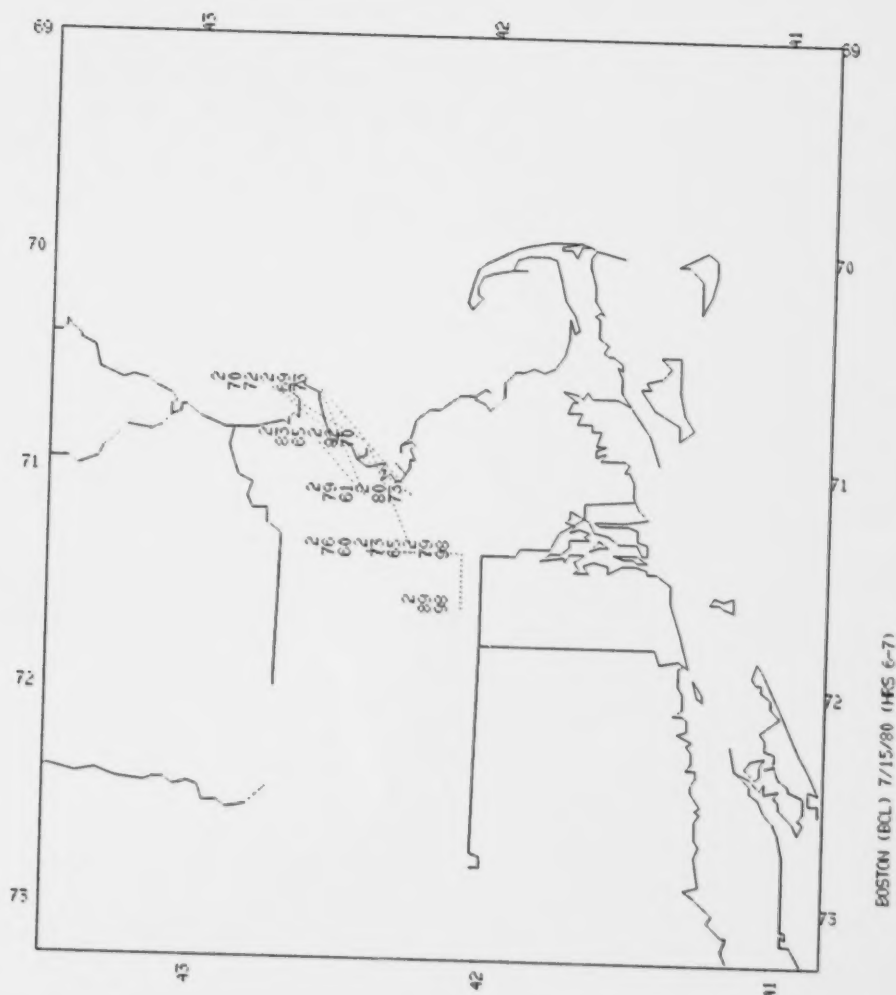
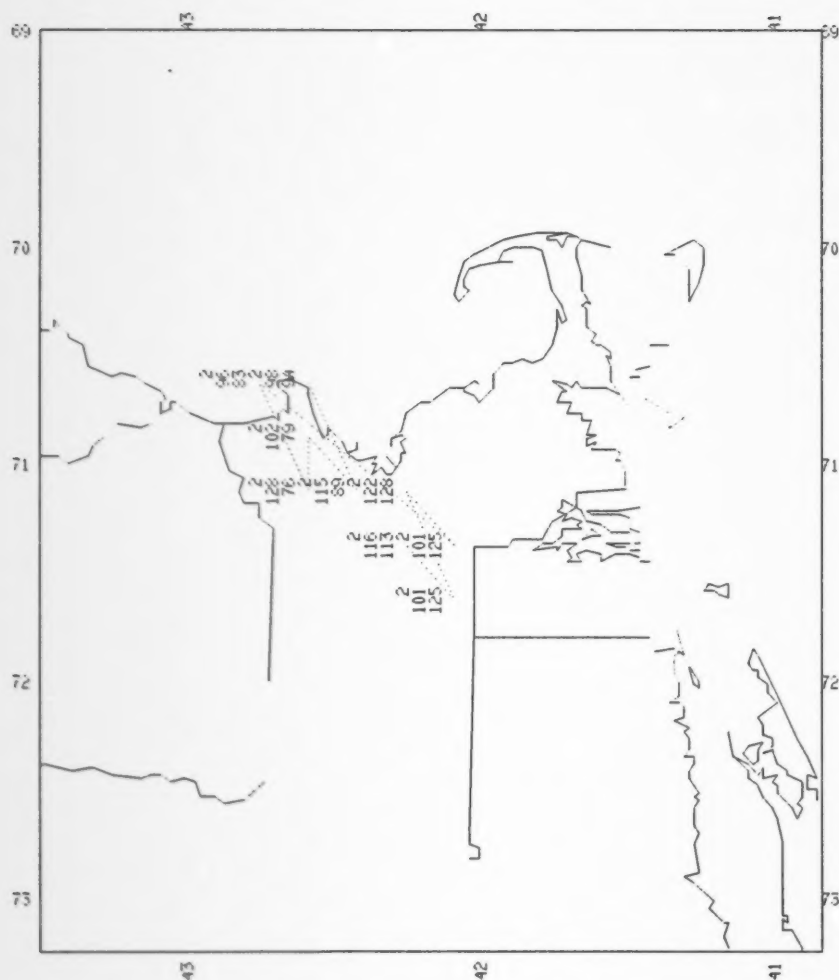


Figure 8.54. Time series of O_3 data from flight on July 31, 1980 in Pittsburgh, PA area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.



BOSTON (BCL) 7/15/80 (HFS 6-7)

Figure 8.55. Geographical distribution of selected O_3 data from flight on July 15, 1980 in Boston, MA area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).



BOSTON (BCL) 7/15/80 (HFS 10-11)

WINCCW extent - rows 18:33 cols 44:60

Figure 8.55 (cont.)



BOSTON (BLL) 7/15/80 (HRS 14-16)

HONEOH extent - rows 18:53 cols 44:80

Figure 8.55 (cont.)

AIRCRAFT - BOSTON AREA JULY 15, 1980 (BCL)

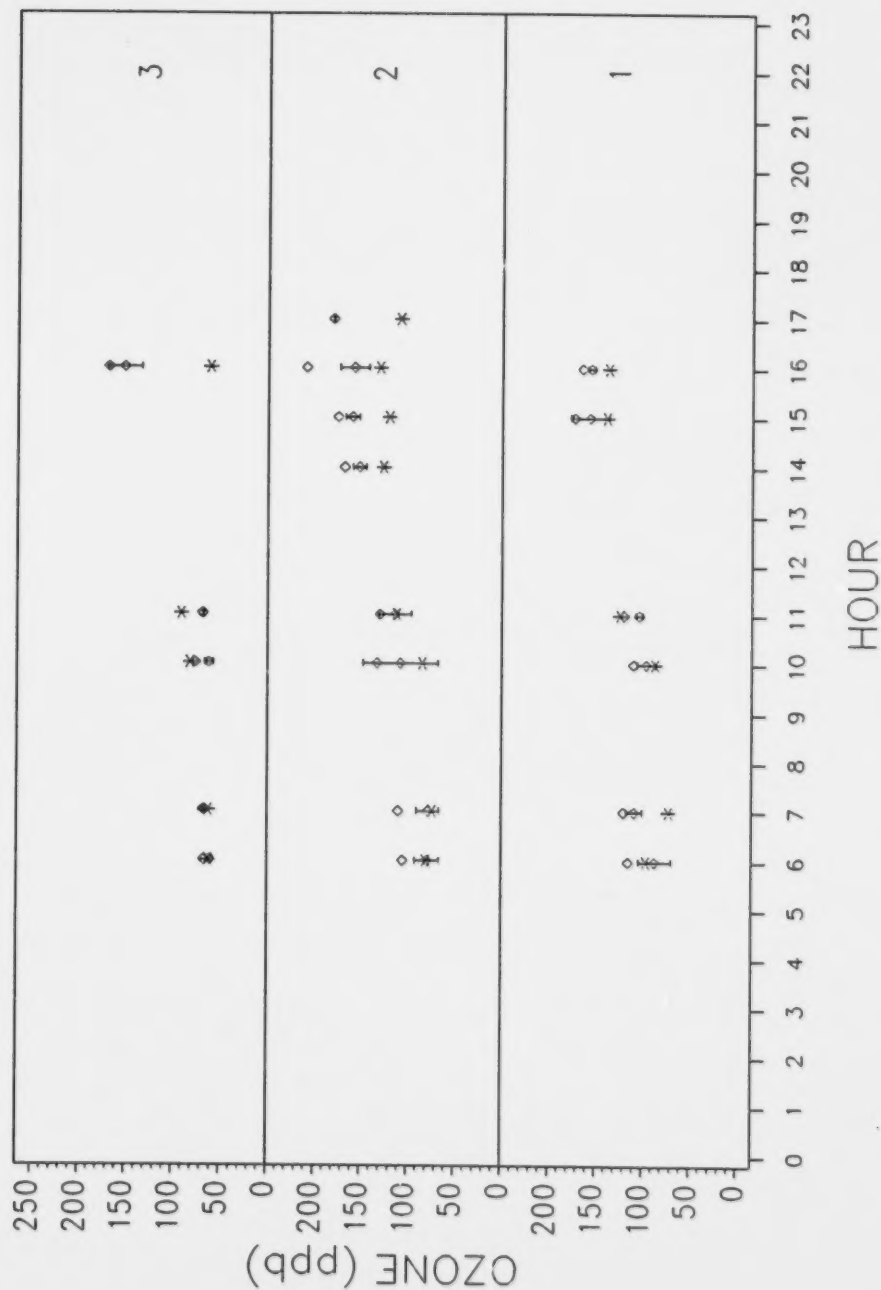


Figure 8.56. Time series of O_3 data from flight on July 15, 1980 in Boston, MA area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

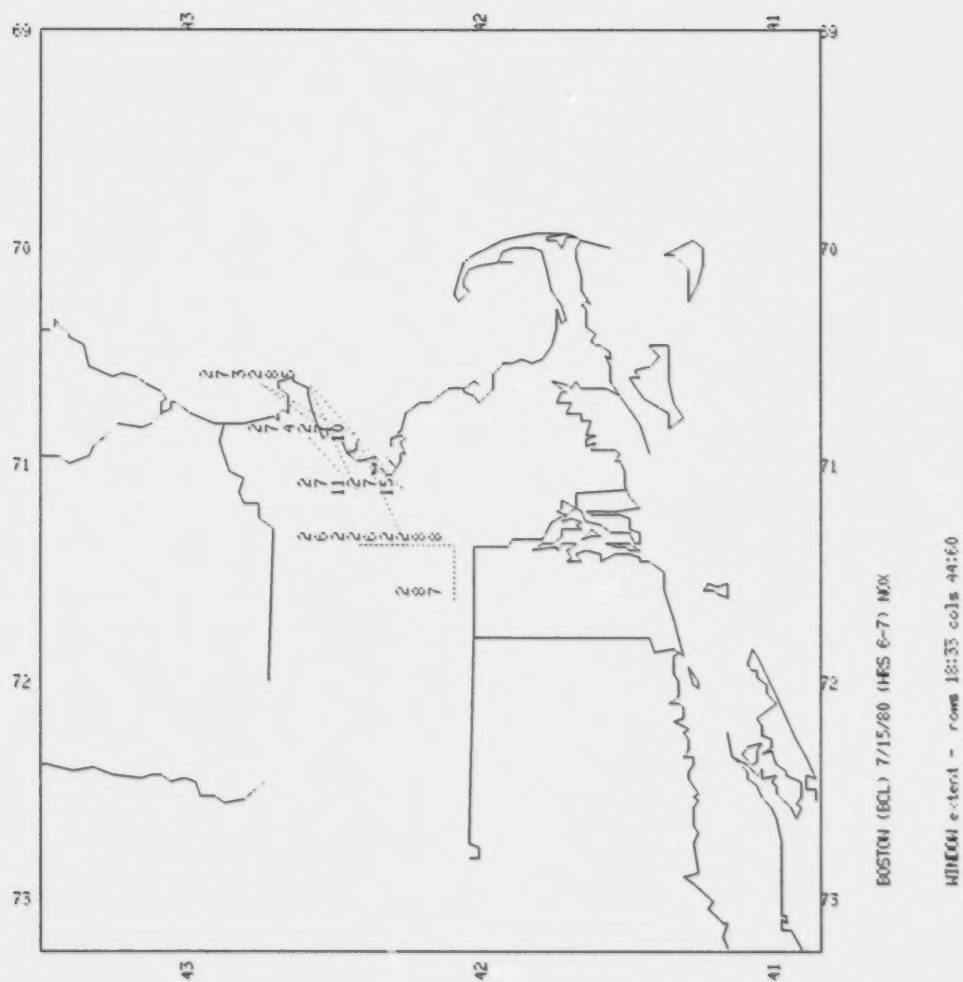
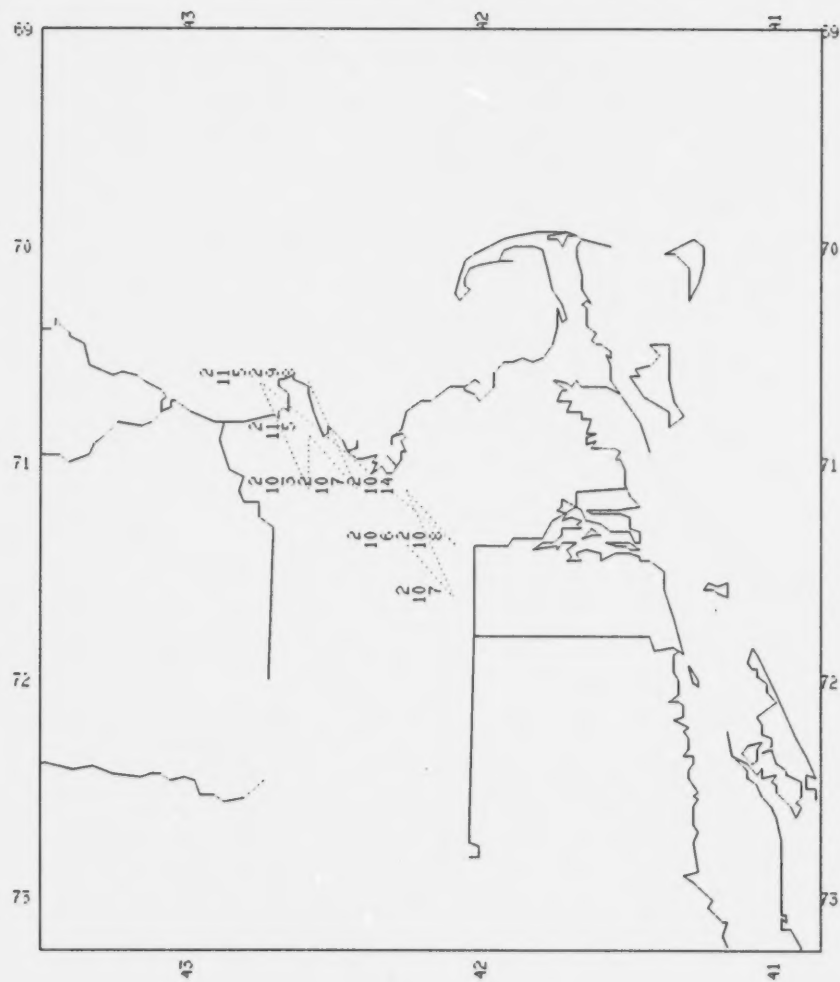


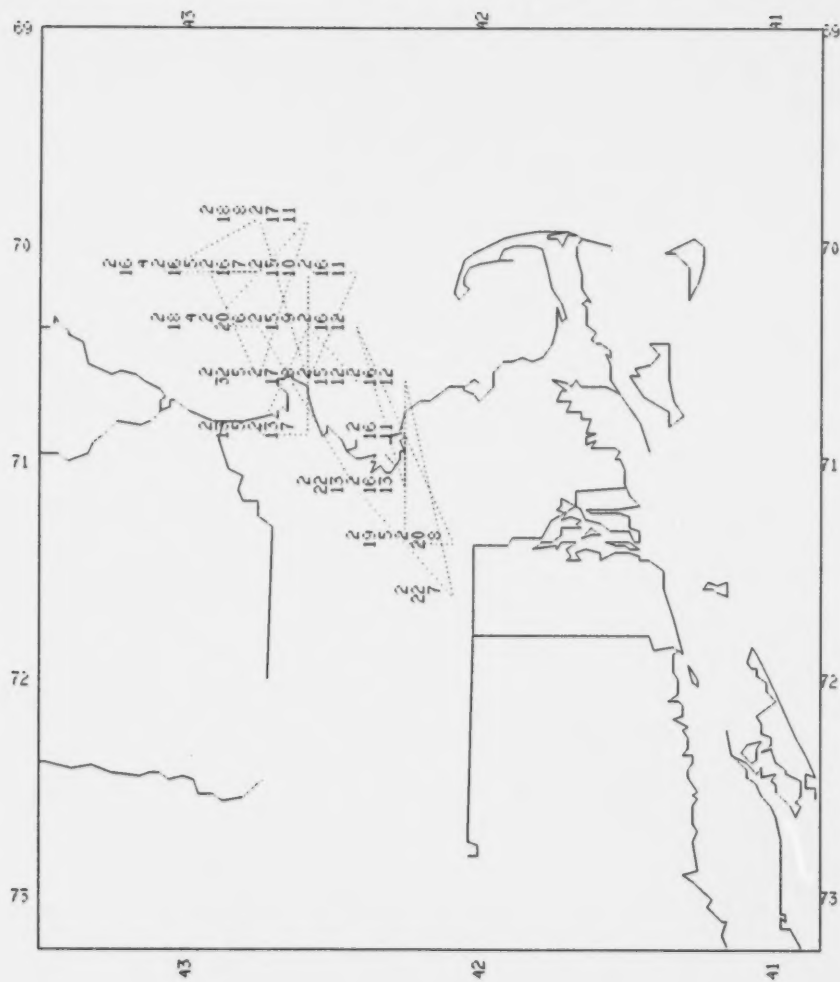
Figure 8.57. Geographical distribution of selected NO_x data from flight on July 15, 1980 in Boston, MA area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).



BOSTON (ELL) 7/15/80 (HRS 10-11) INOX

WINDOW extent - rows 18:33 cols 44:60

Figure 8.57 (cont.)



BOSTON (BCL) 7/15/80 (HRS 14-16) NEX

WIMCO extent - rows 18:33 cols 44:60

Figure 8.57 (cont.)

AIRCRAFT - BOSTON AREA JULY 15, 1980 (BCL)

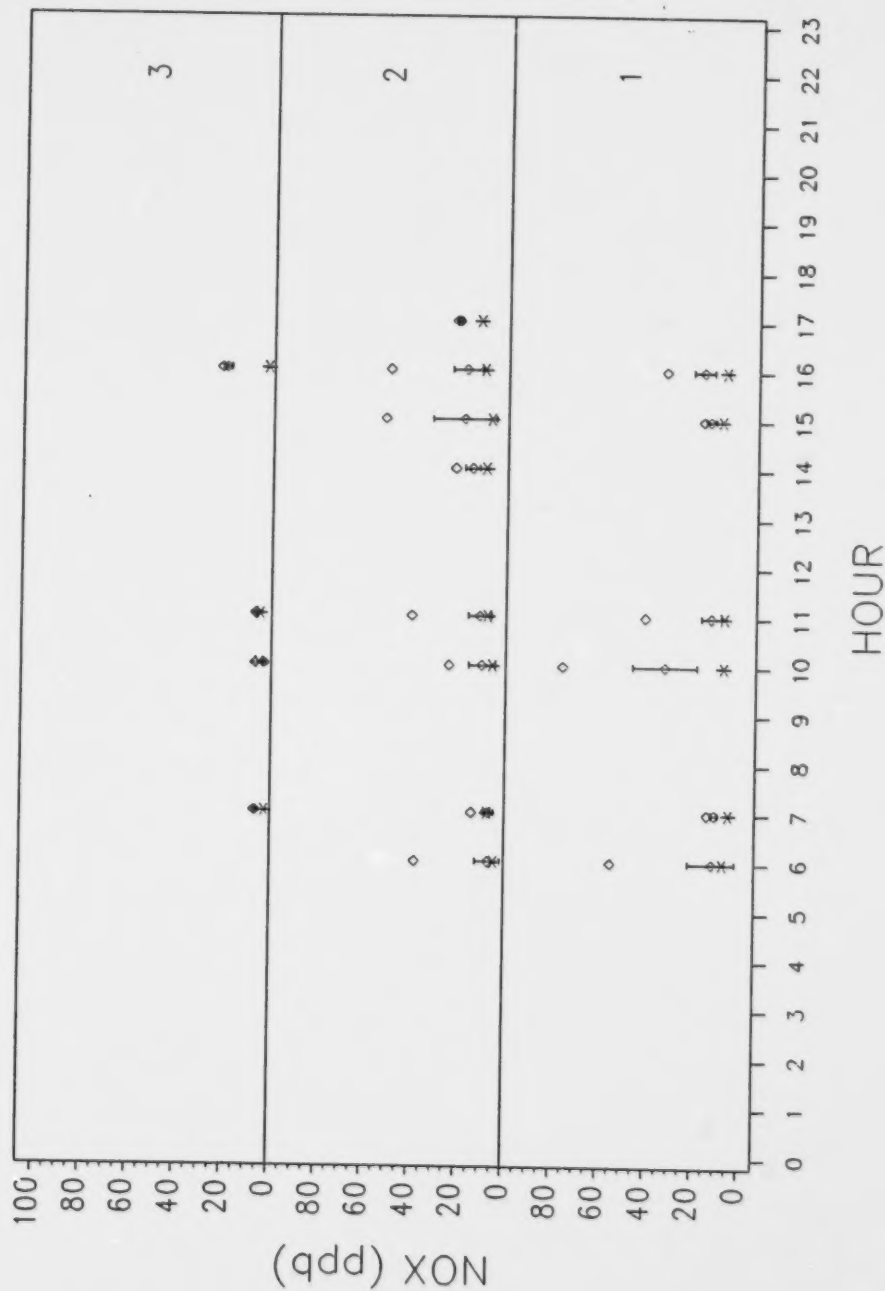


Figure 8.58. Time series of NO_x data from flight on July 15, 1980 in Boston, MA area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

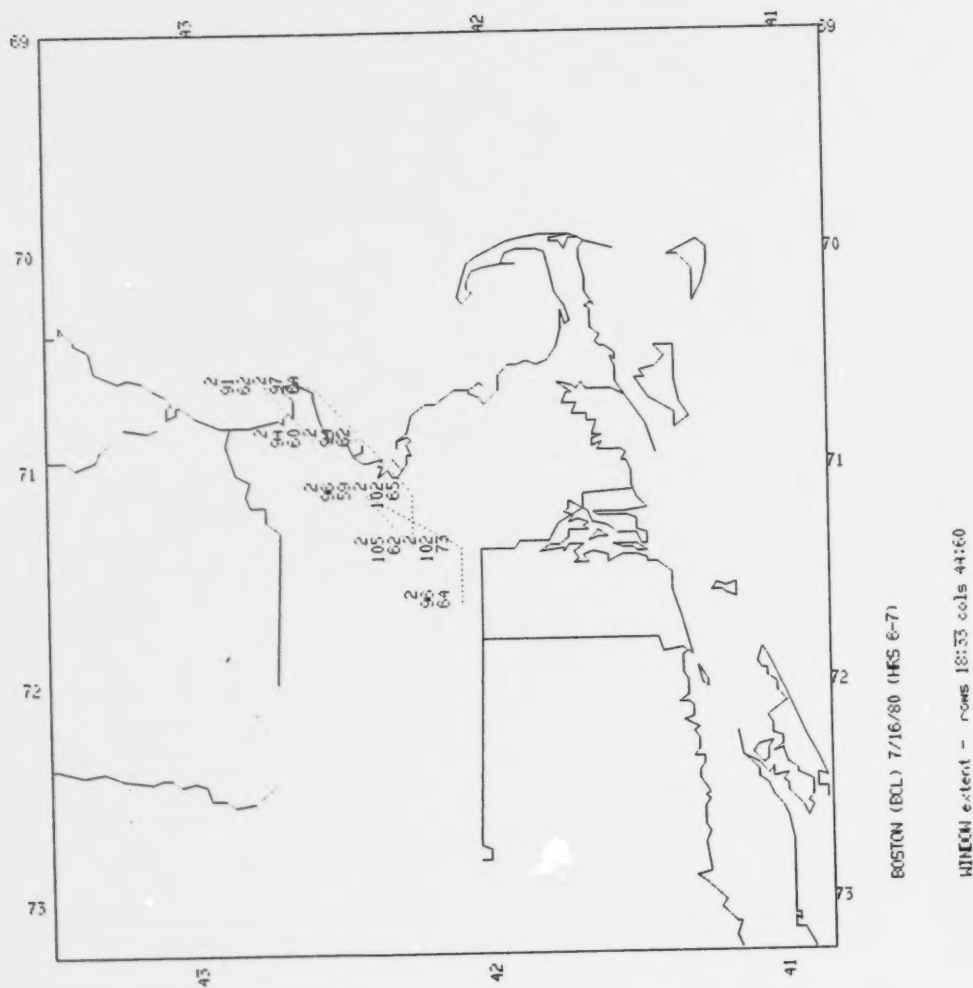
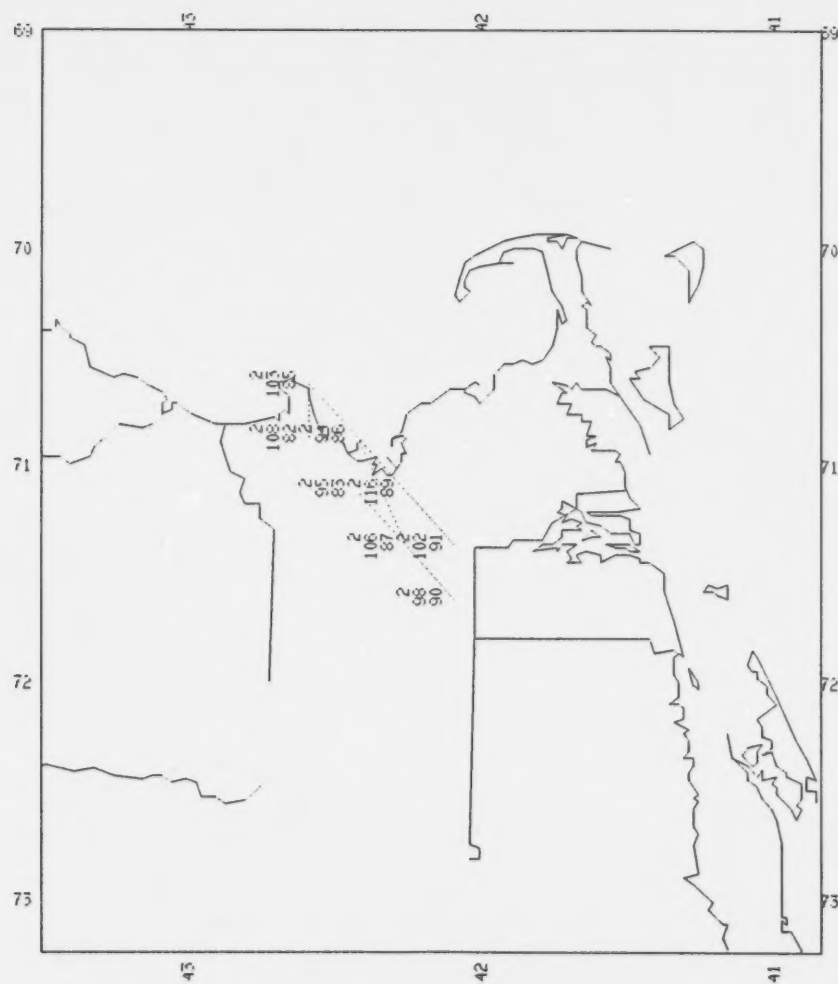


Figure 8.59. Geographical distribution of selected O₃ data from flight on July 16, 1980 in Boston, MA area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).



BOSTON (ECL) 7/16/80 (HRS 10-11)

NINOW extent - rows 18:33 cols 44:60

Figure 8.59 (cont.)

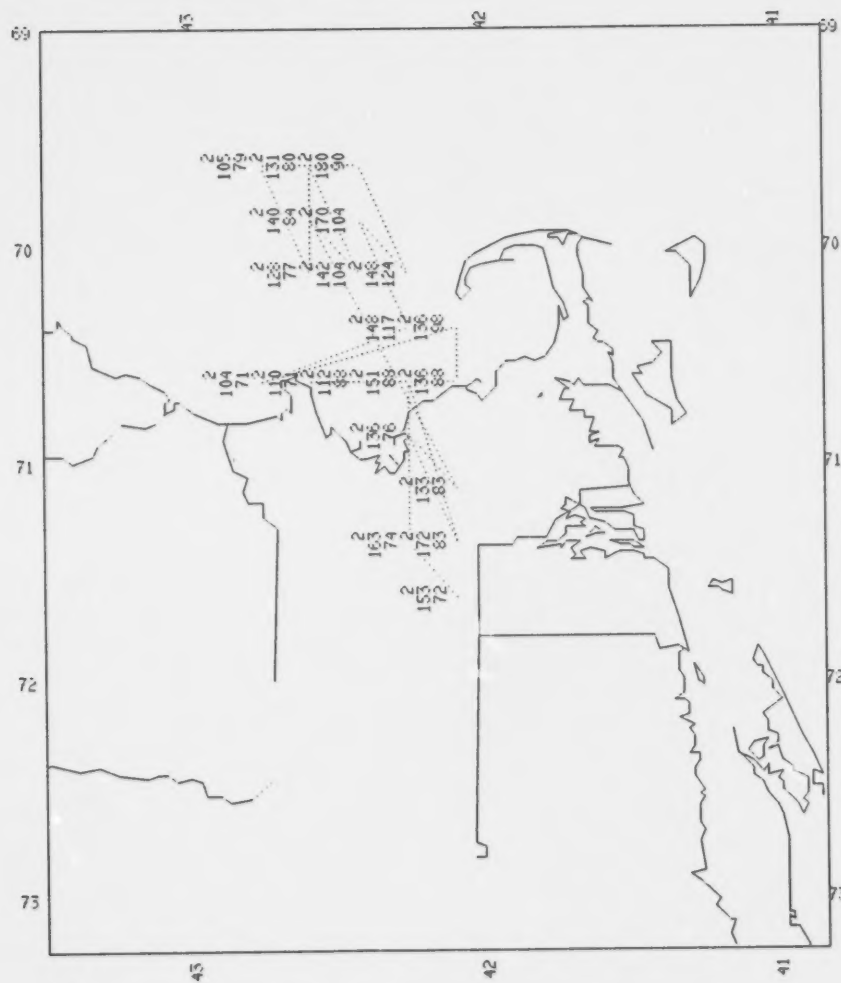


Figure 8.59 (cont.)

AIRCRAFT - BOSTON AREA JULY 16, 1980 (BCL)

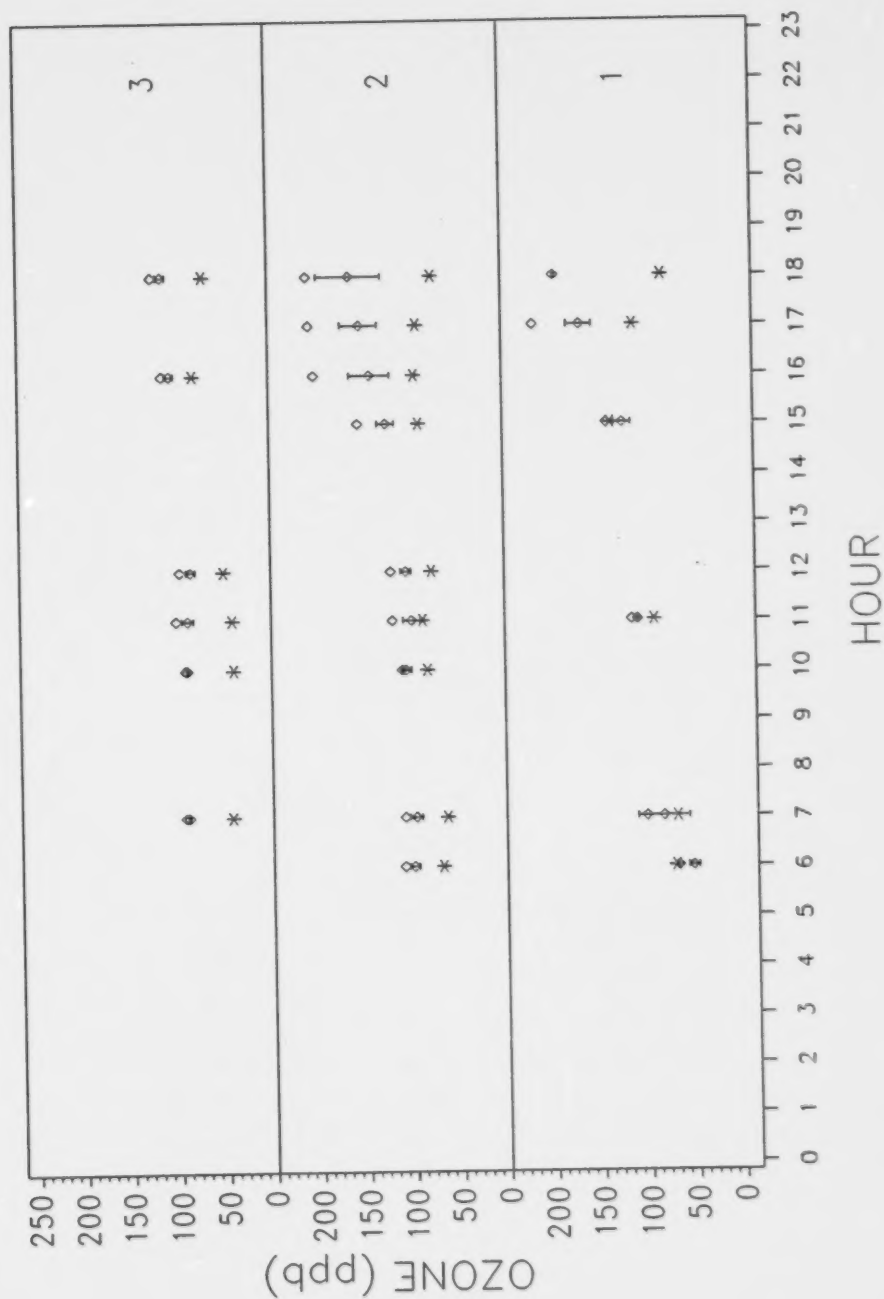
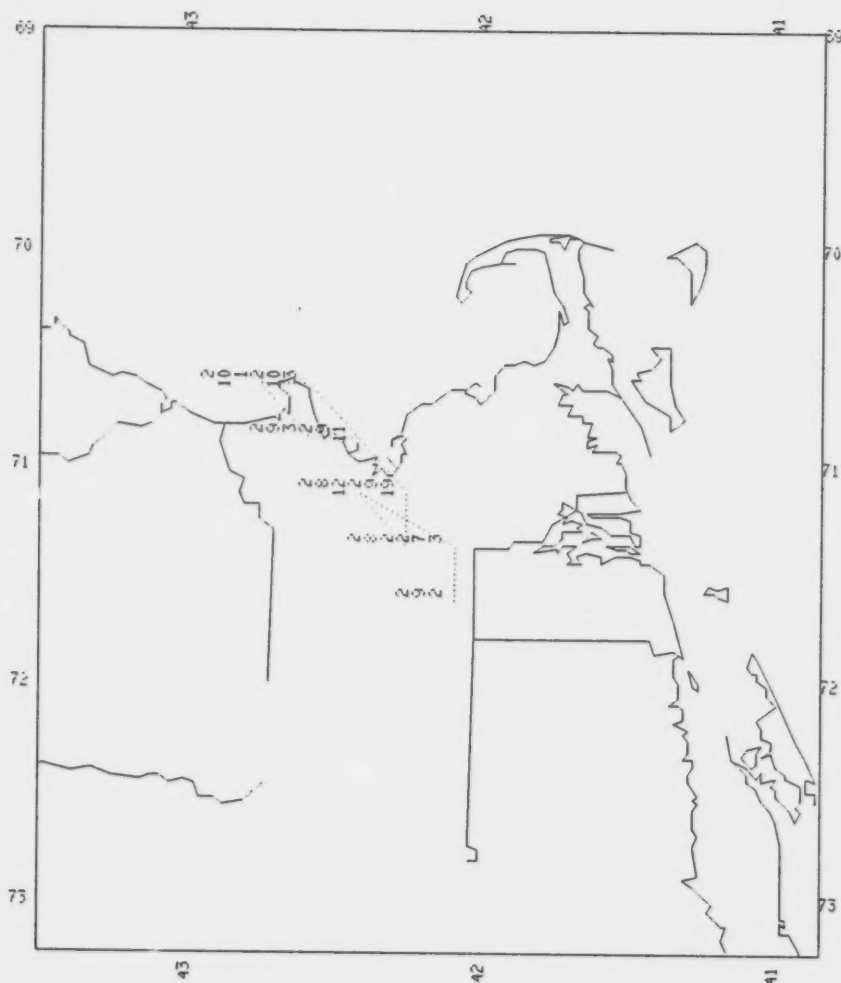


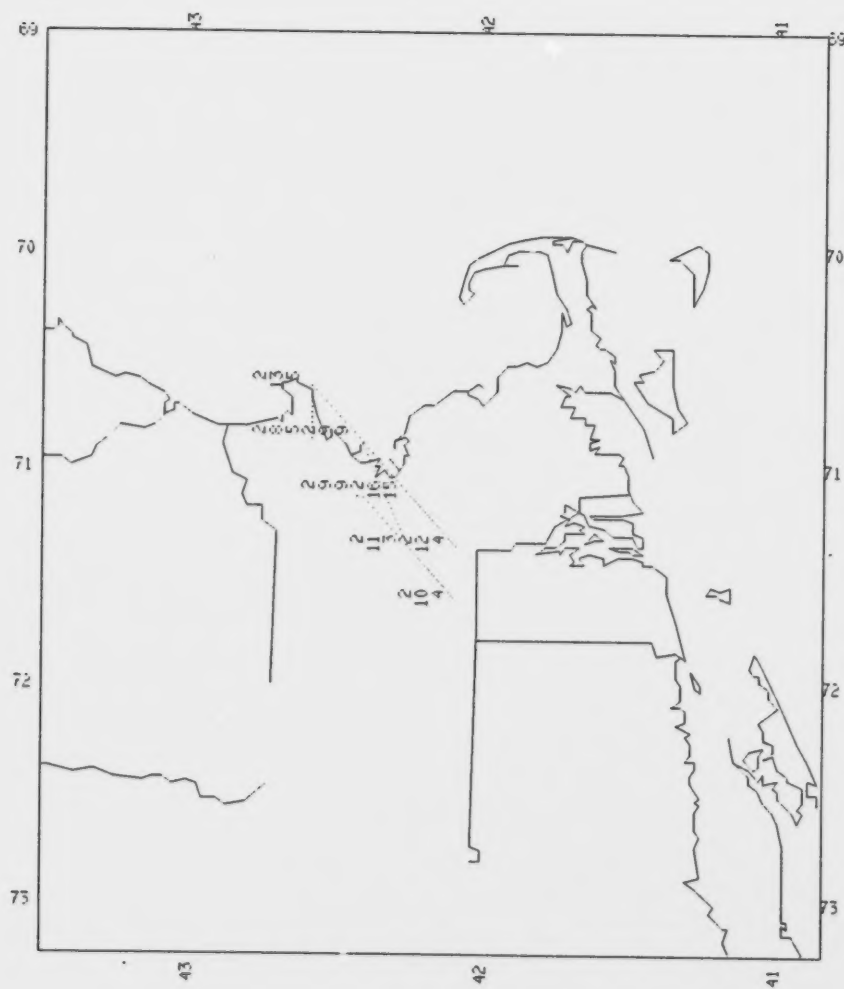
Figure 8.60. Time series of O_3 data from flight on July 16, 1980 in Boston, MA area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.



BOSTON (BCL) 7/16/80 (HFS 6-7) NOX

WINDMILL extent - rows 18:33 cols 44:60

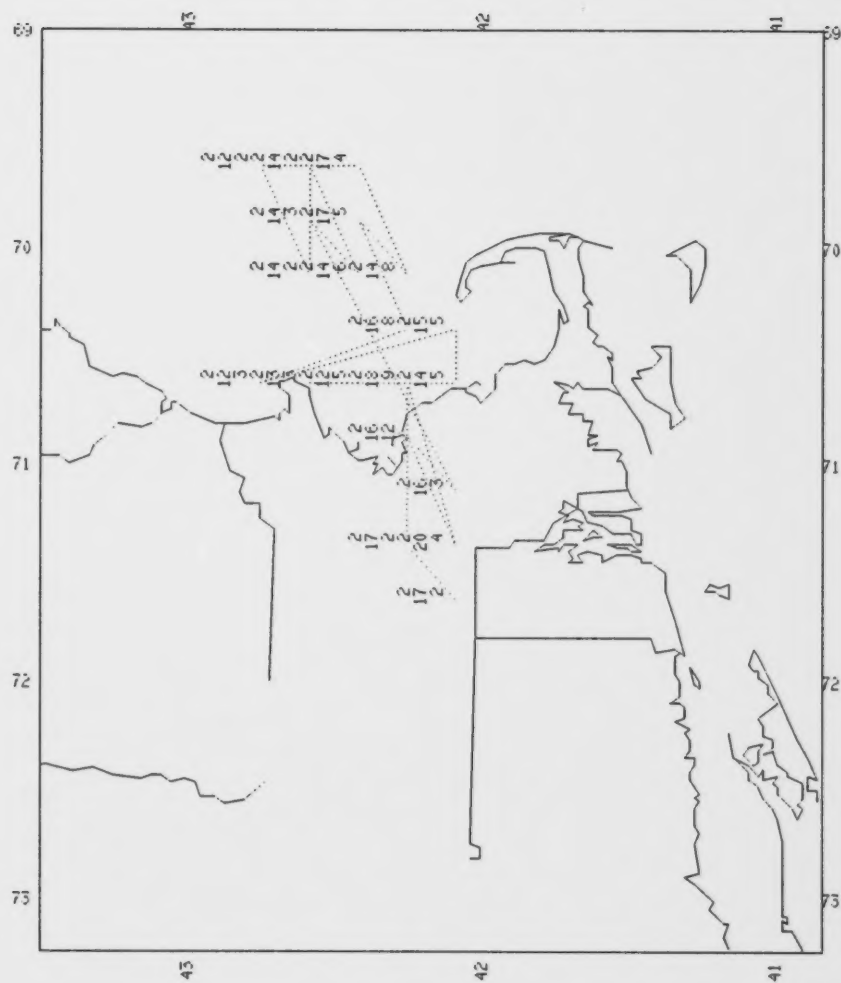
Figure 8.61. Geographical distribution of selected NO_x data from flight on July 16, 1980 in Boston, MA area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).



BOSTON (ECL) 7/16/80 (HRS 10-11) NOX

WHEON extent - rows 18:53 cols 44:60

Figure 8.61 (cont.)



BOSTON (ECL) 7/16/80 (HFS 15-18) NOX

WINDCHILL extent - rows 18:33 cols 44:60

Figure 8.61 (cont.)

AIRCRAFT - BOSTON AREA JULY 16, 1980 (BCL)

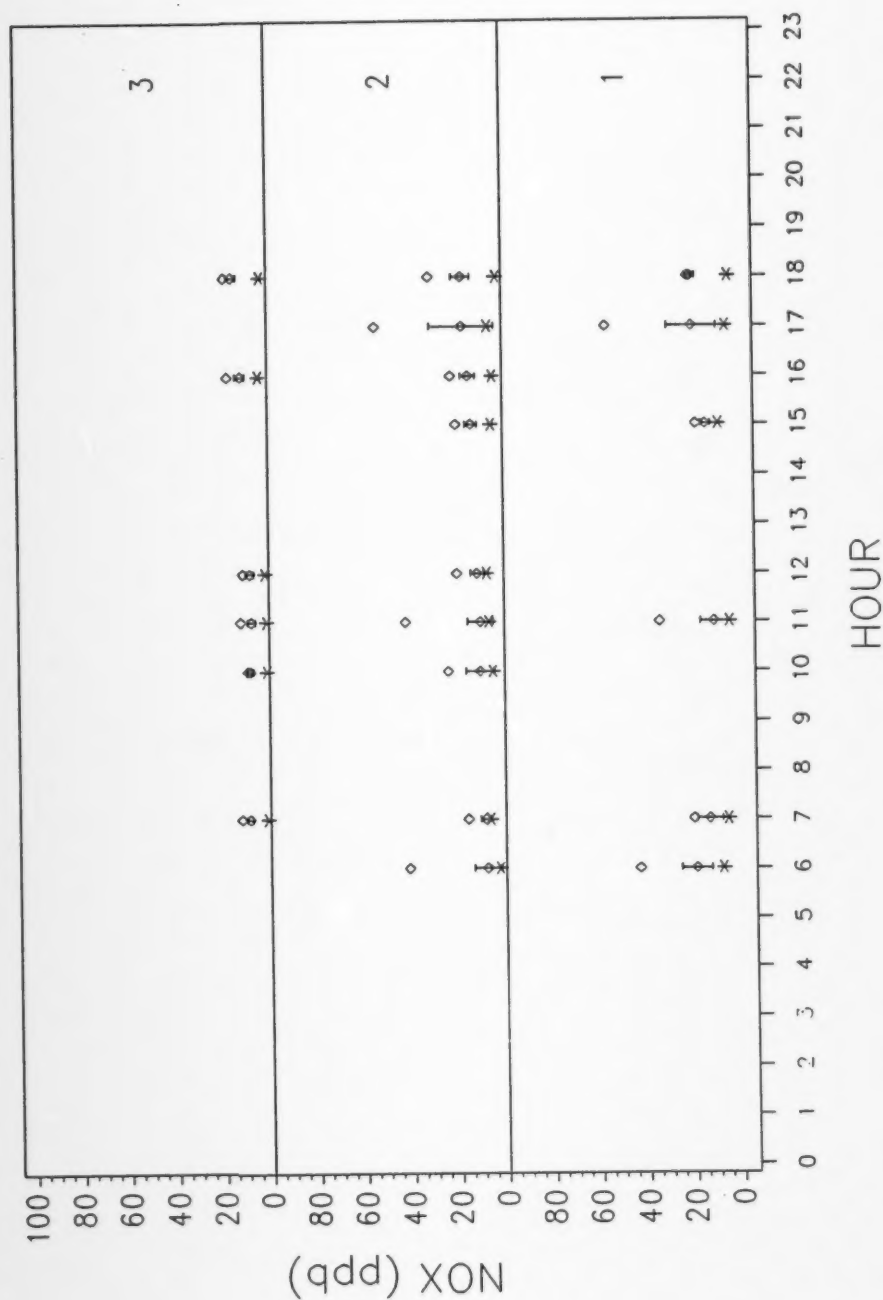
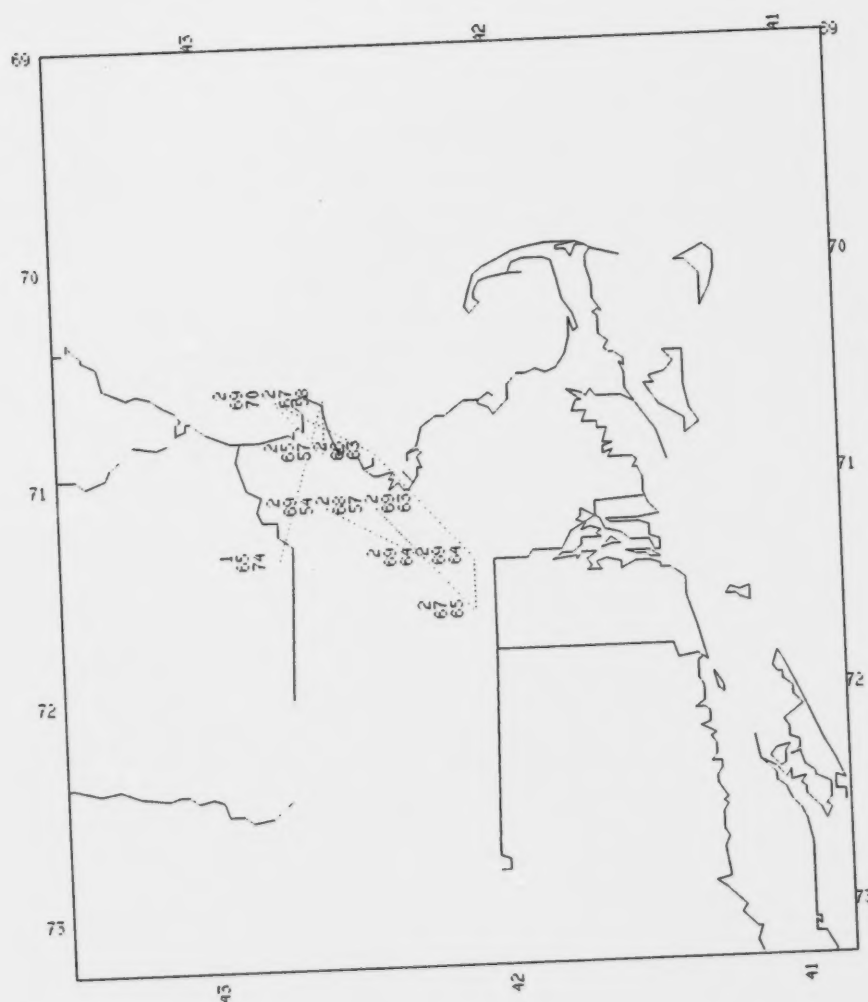


Figure 8.62. Time series of NO_x data from flight on July 16, 1980 in Boston, MA area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.



BOSTON (ECL) 8/08/80 (HRS 5-7)

WUECH extent - rows 18:33 cols 44:60

Figure 8.63. Geographical distribution of selected O₃ data from flight on Aug. 8, 1980 in Boston, MA area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

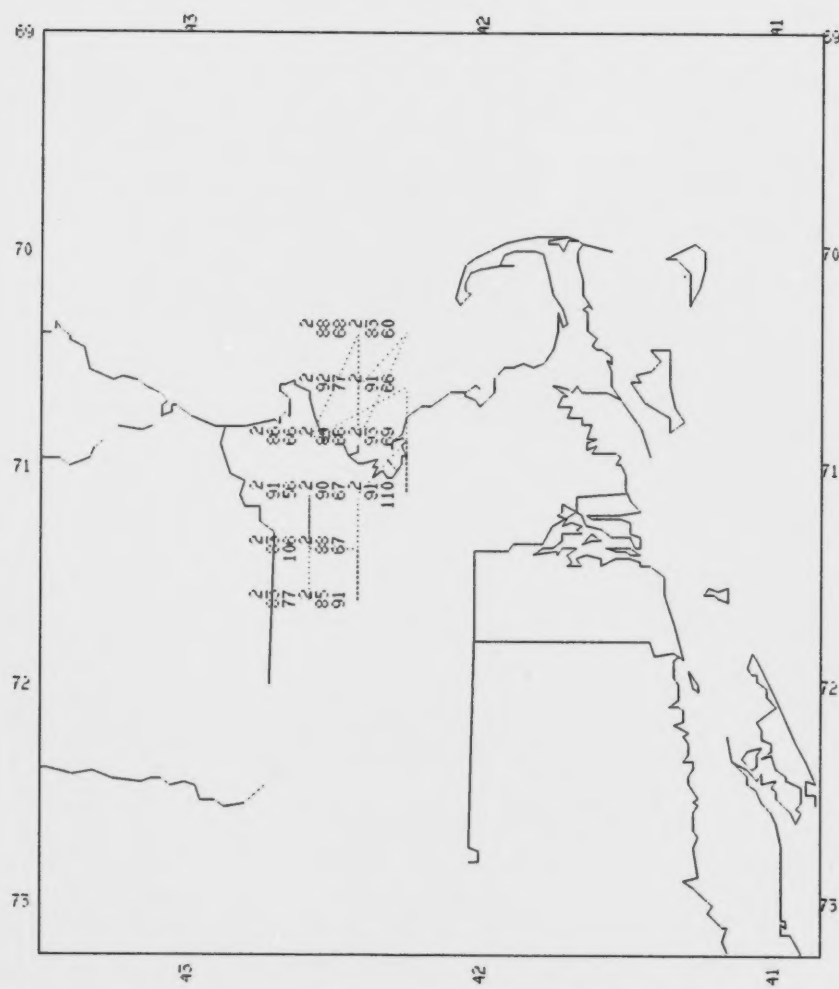
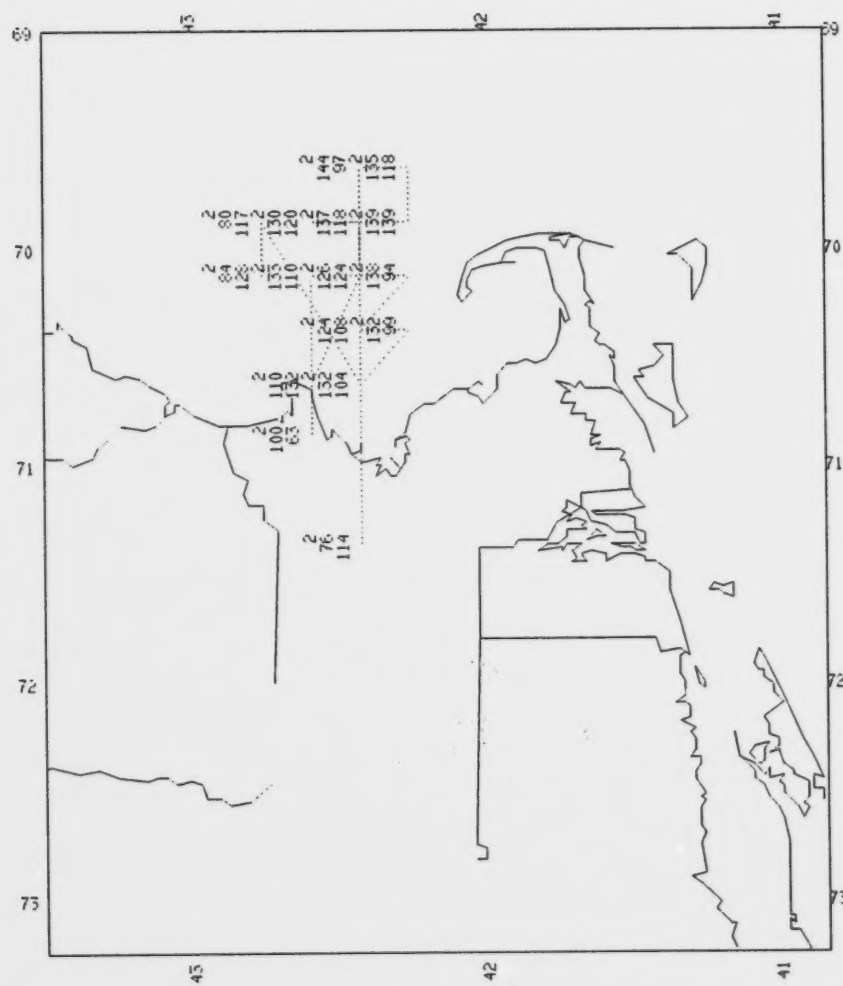


Figure 8.63 (cont.)



BOSTON (ECL) 8/08/80 (HRS 14-16)

WHECO extent - rows 18:33 cols 44:50

Figure 8.63 (cont.)

AIRCRAFT - BOSTON AREA AUGUST 8, 1980 (BCL)

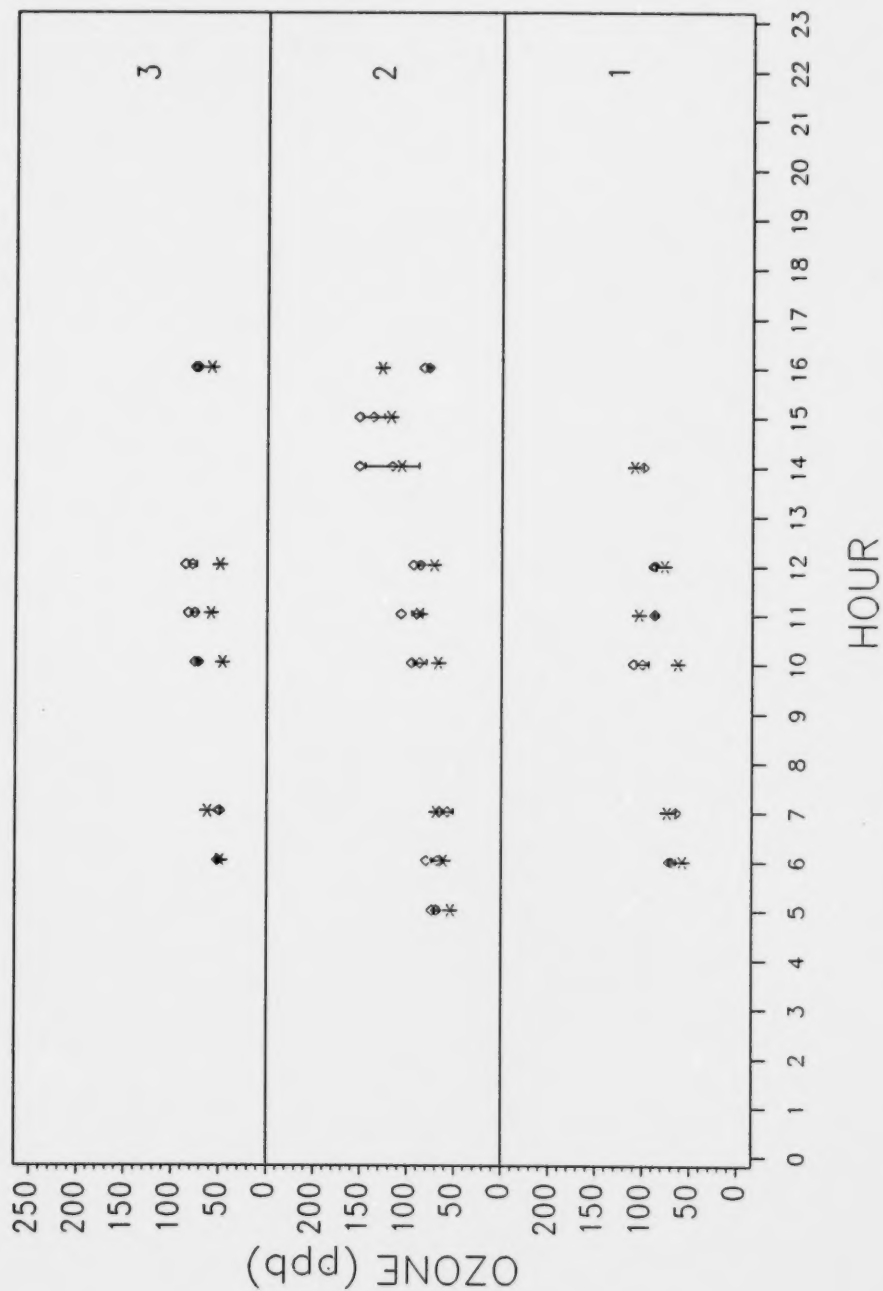


Figure 8.64. Time series of O₃ data from flight on Aug. 8, 1980 in Boston, MA area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

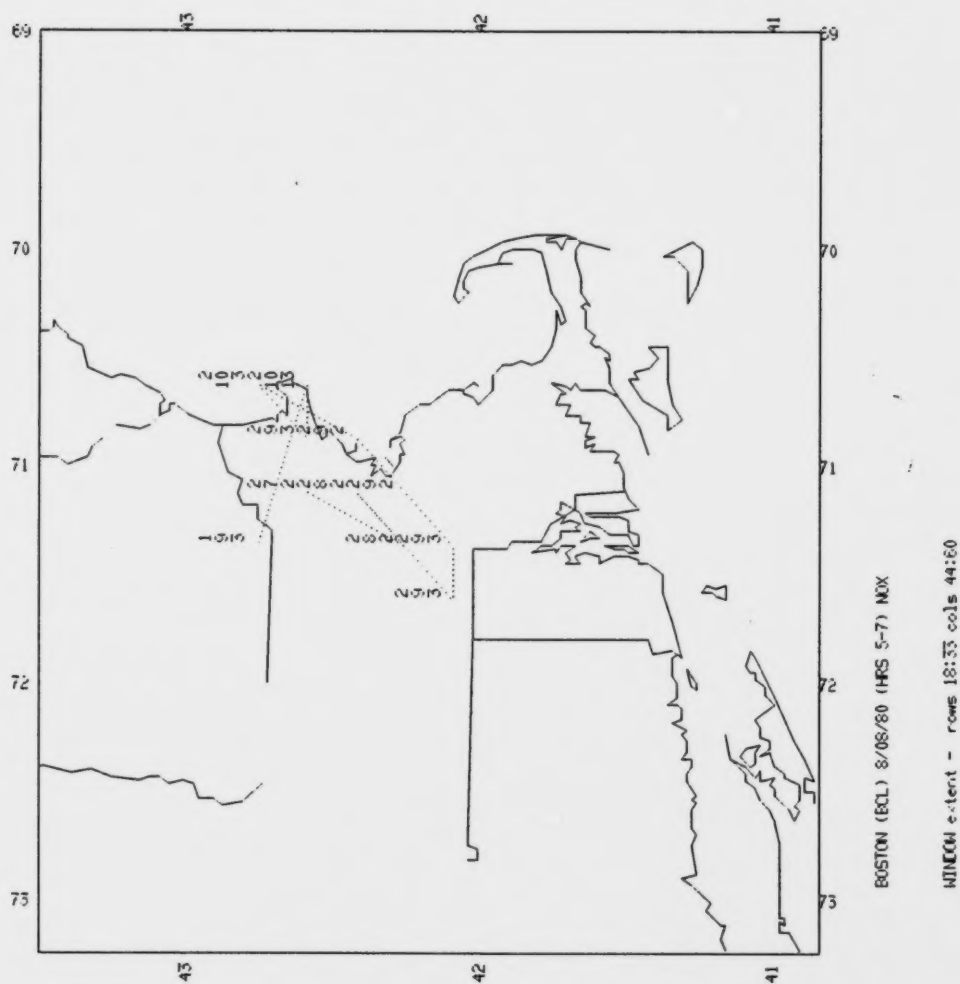
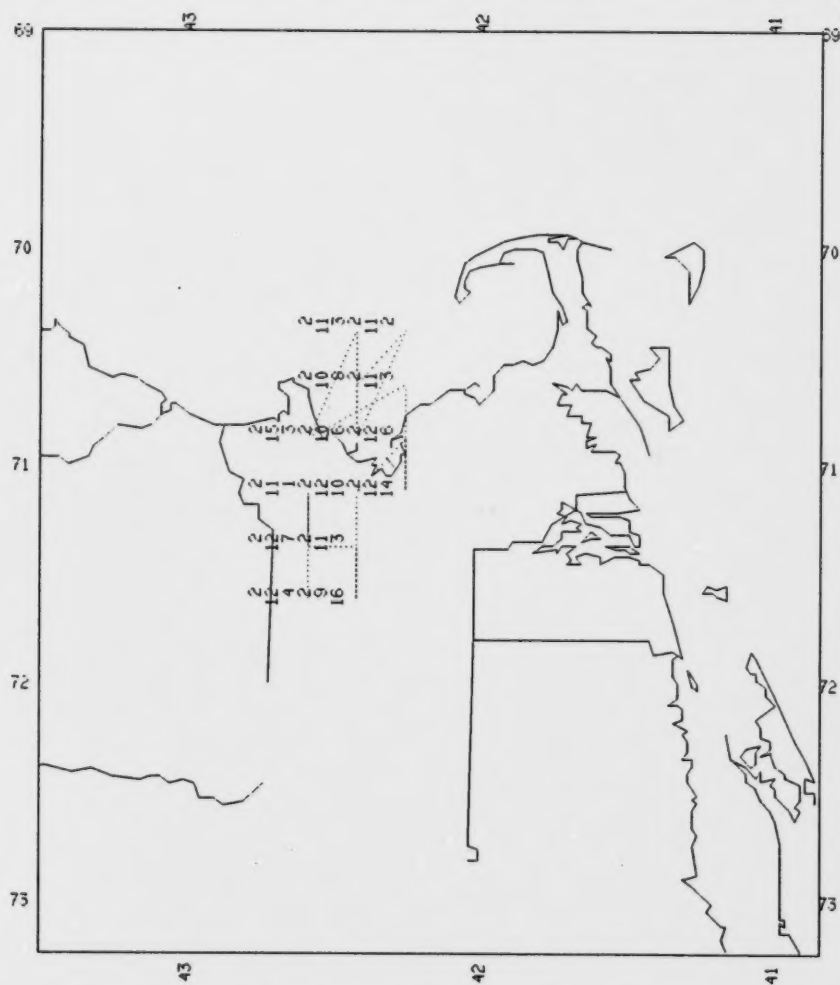


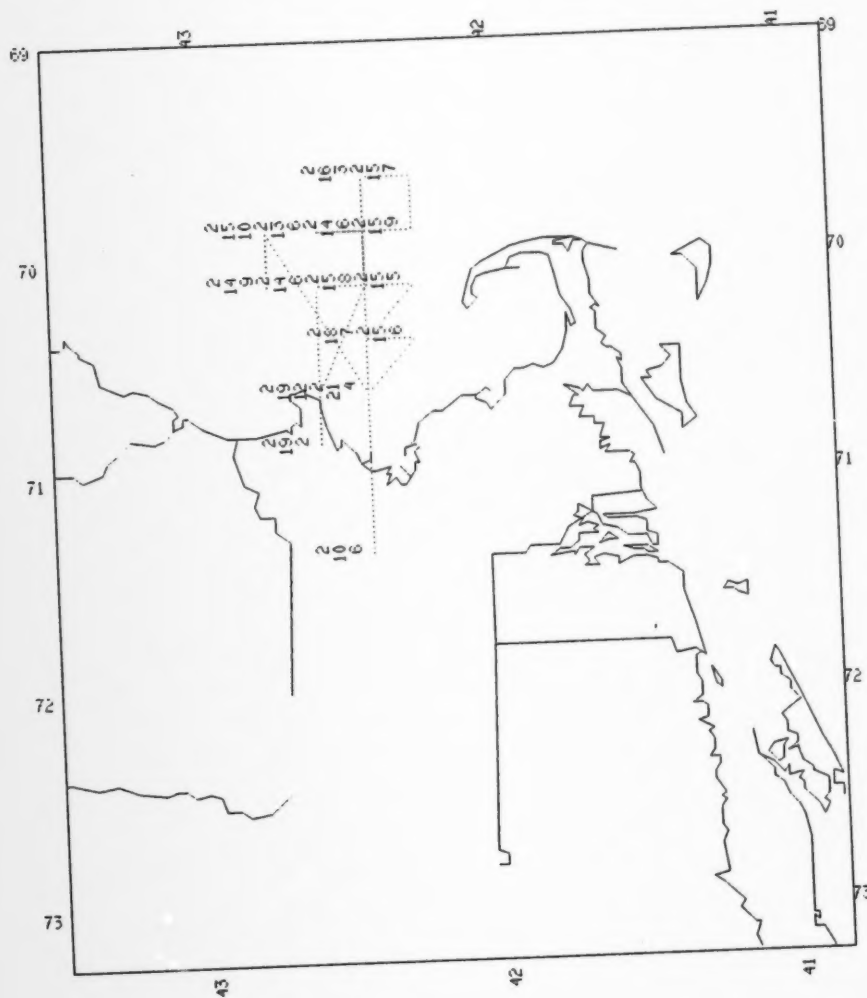
Figure 8.65. Geographical distribution of selected NO_x data from flight on Aug. 8, 1980 in Boston, MA area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).



BOSTON (BCL) 8/08/80 (HRS 10-12) NOX

WINNIX extent - rows 18:33 cols 44:60

Figure 8.65 (cont.)



BOSTON (BCL) 8/08/80 (HRS 14-18) NOX

WINDOWN extent - rows 18:53 cols 44:60

Figure 8.65 (cont.)

AIRCRAFT - BOSTON AREA AUGUST 8, 1980 (BCL)



Figure 8.66. Time series of NO_x data from flight on Aug. 8, 1980 in Boston, MA area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

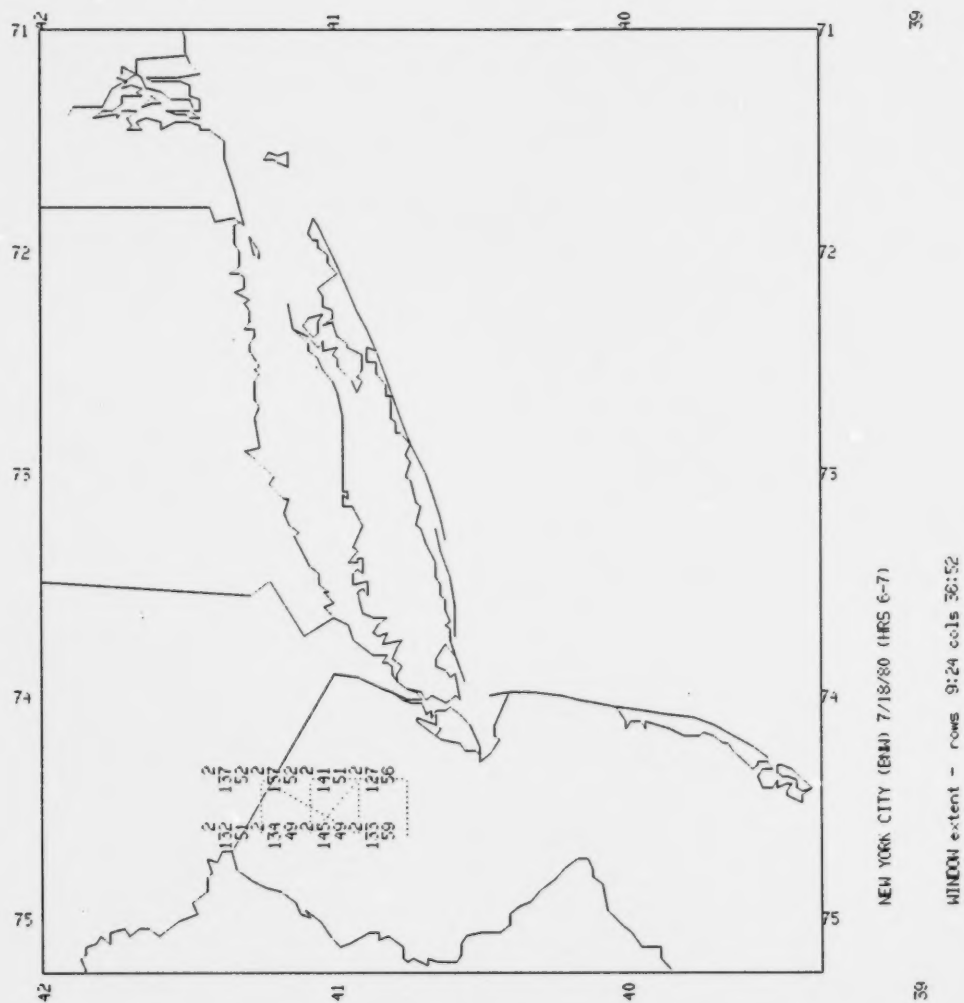
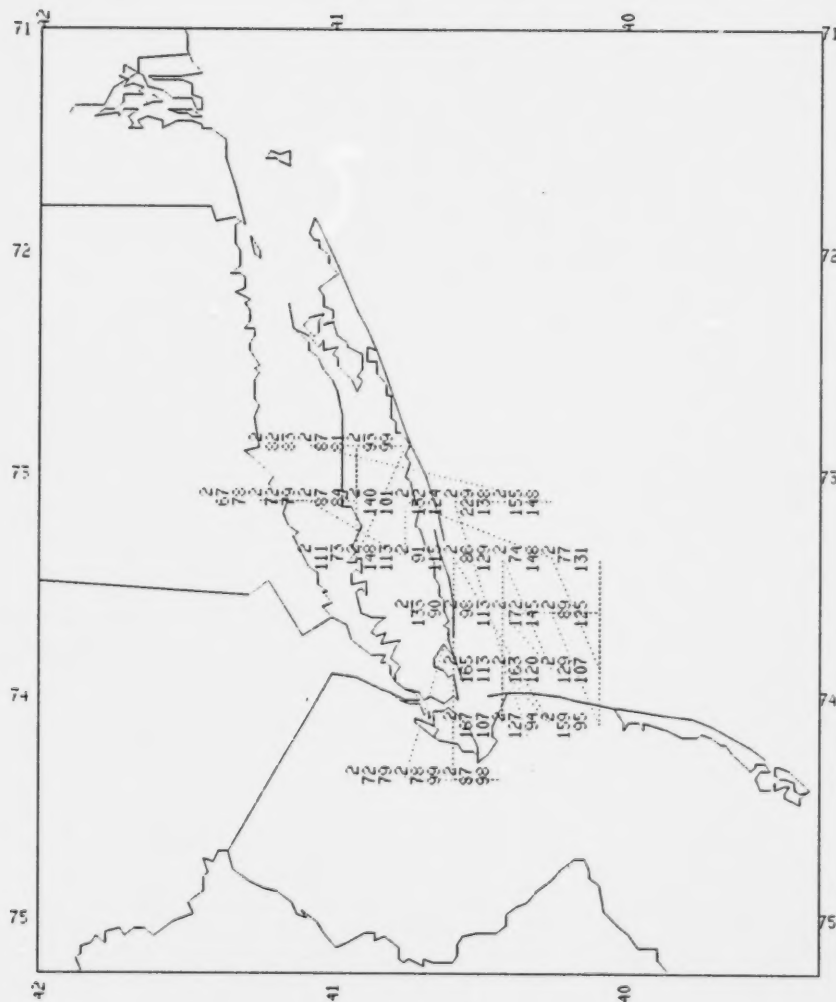


Figure 8.67. Geographical distribution of selected O₃ data from flight on July 18, 1980 in New York, NY area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).



NEW YORK CITY (END) 7/18/80 (HRS 12-19)

WINDOW extent - rows 9:24 cols 38:52

Figure 8.67 (cont.)

AIRCRAFT - NEW YORK CITY AREA JULY 18, 1980 (BNW)

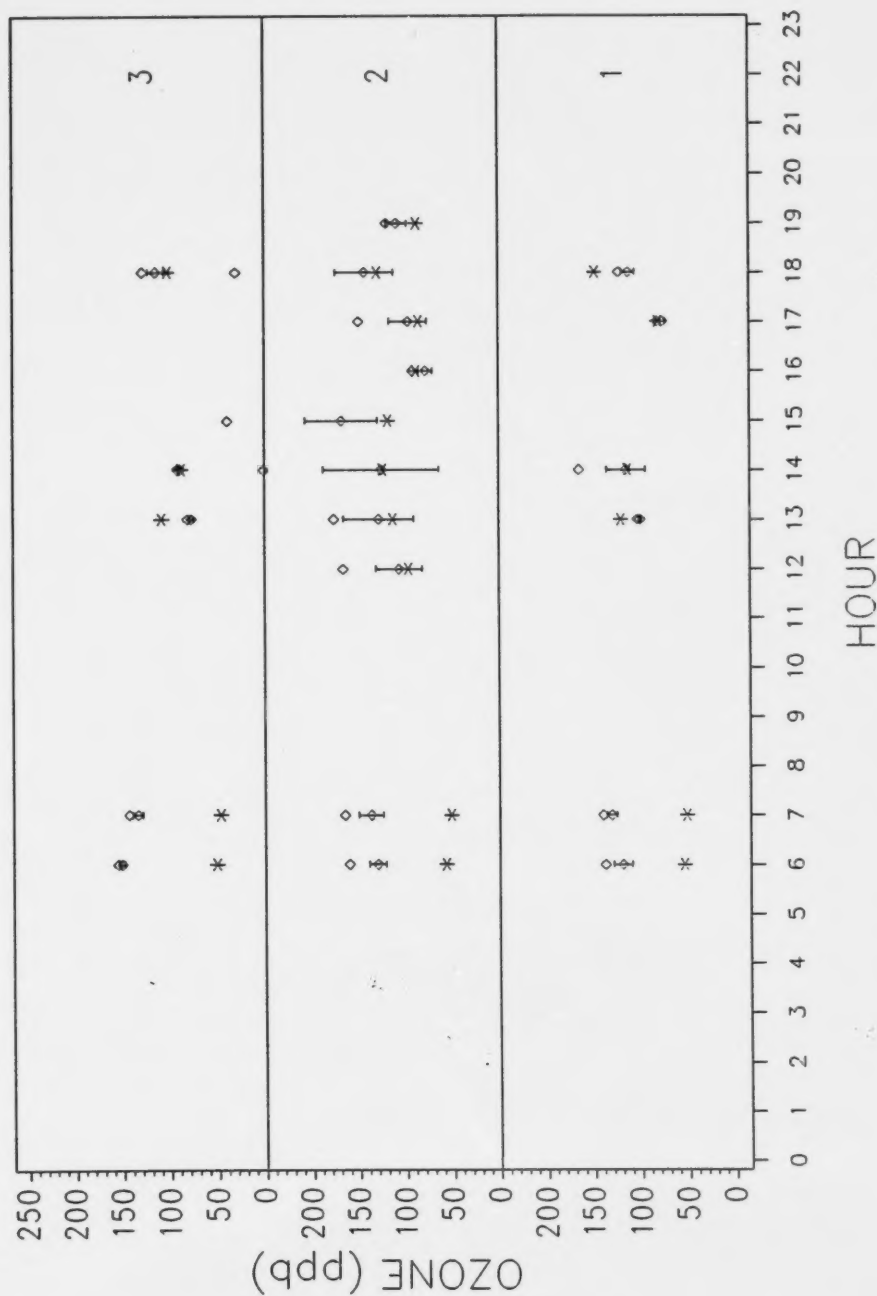


Figure 8.68. Time series of O₃ data from flight on July 18, 1980 in New York, NY area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

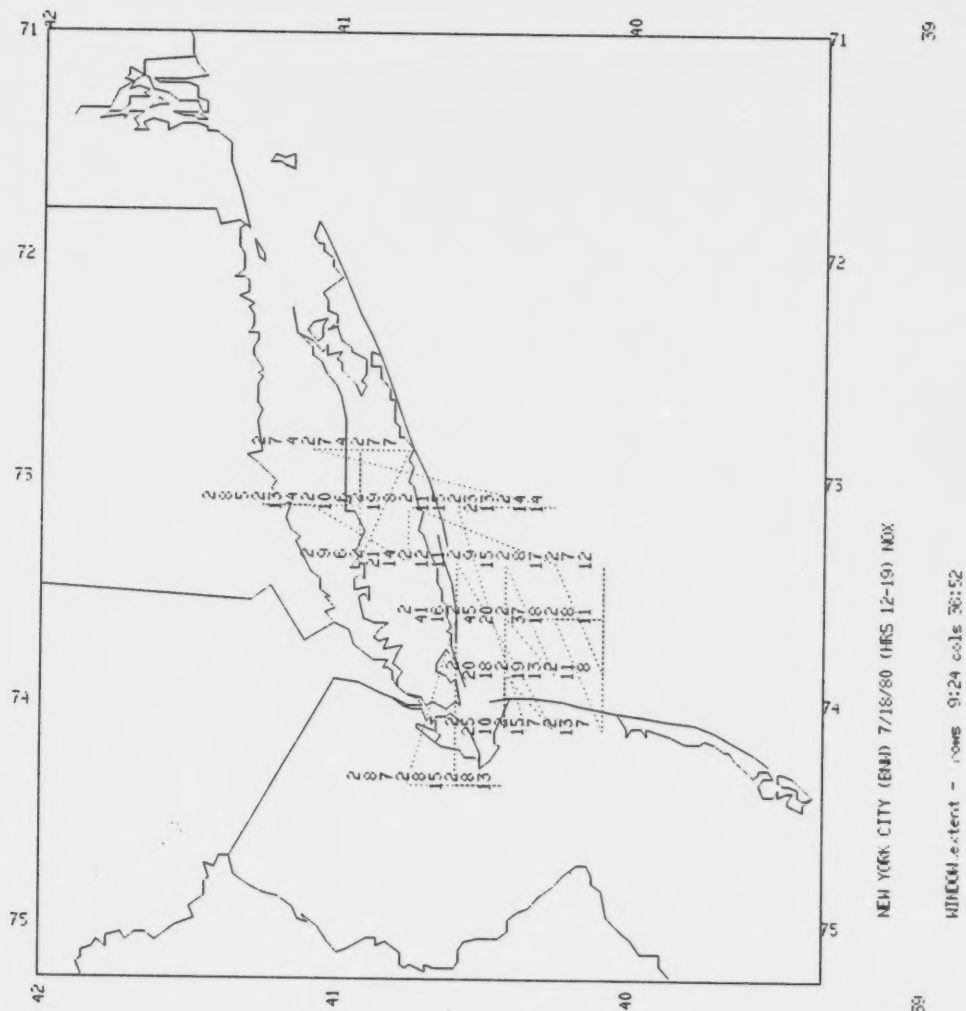


Figure 8.69. Geographical distribution of selected NO_x data from flight on July 18, 1980 in New York, NY area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - NEW YORK CITY AREA JULY 18, 1980 (BNW)

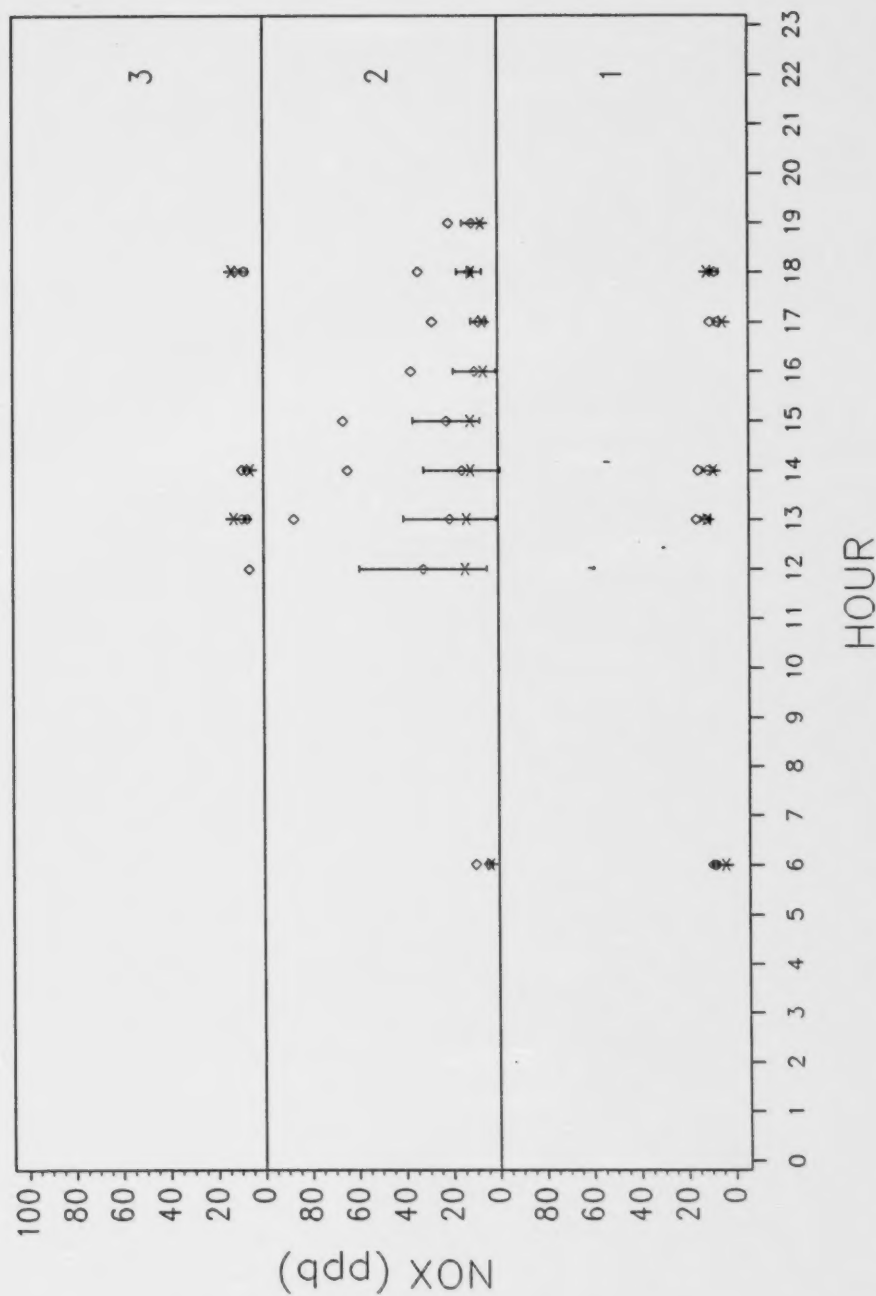


Figure 8.70. Time series of NO_x data from flight on July 18, 1980 in New York, NY area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

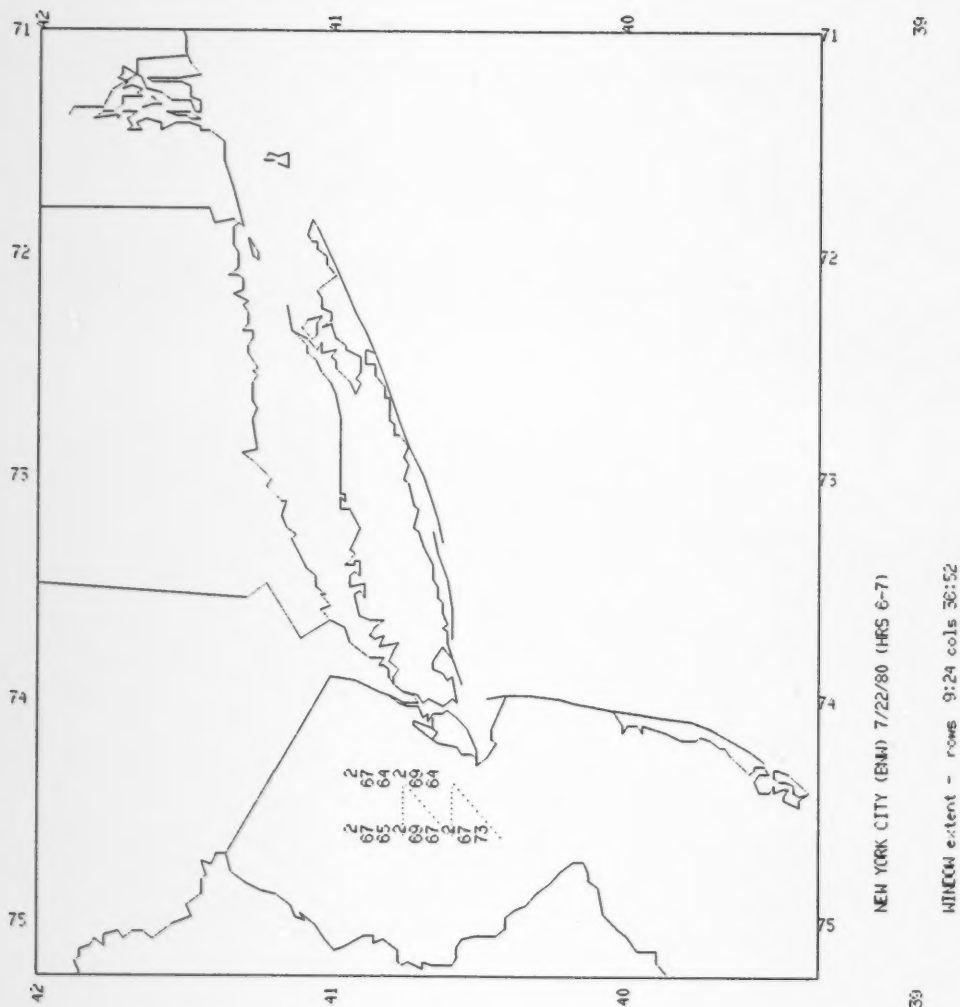
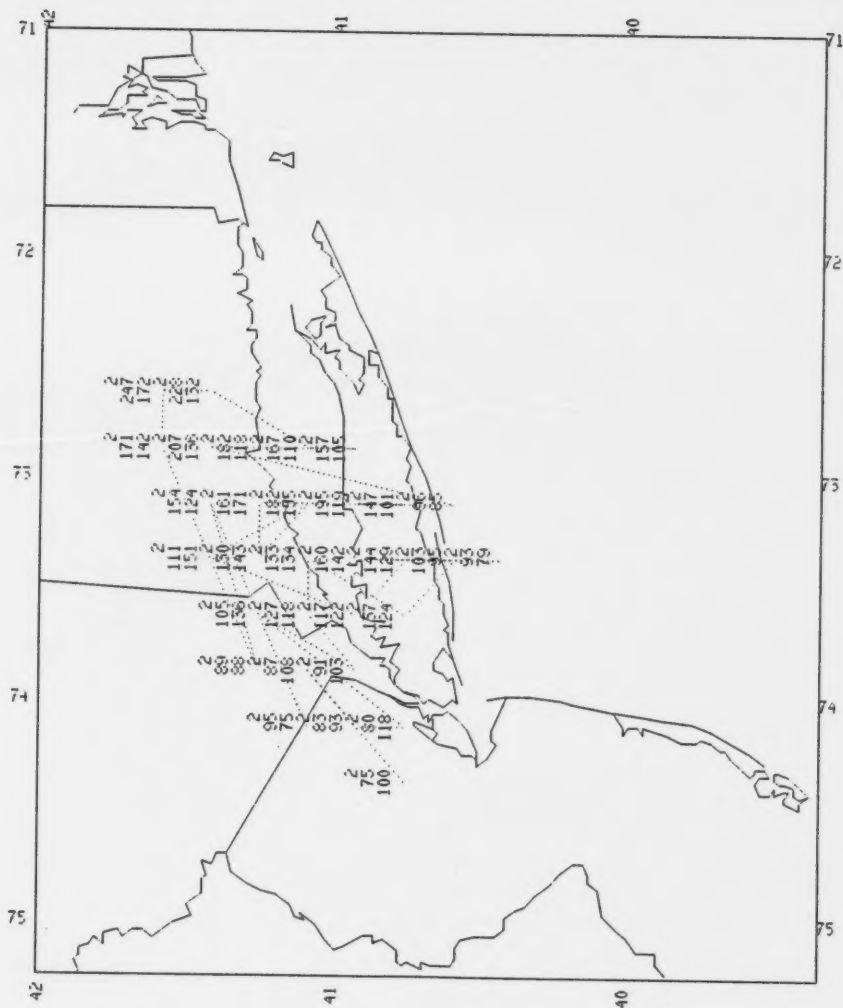


Figure 8.71. Geographical distribution of selected O_3 data from flight on July 22, 1980 in New York, NY area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).



NEW YORK CITY (BN) 7/22/80 (HRS 12-18)

WINDOW extent - rows 9:24 cols 36:52

Figure 8.71 (cont.)

AIRCRAFT - NEW YORK CITY AREA JULY 22, 1980 (BNW)

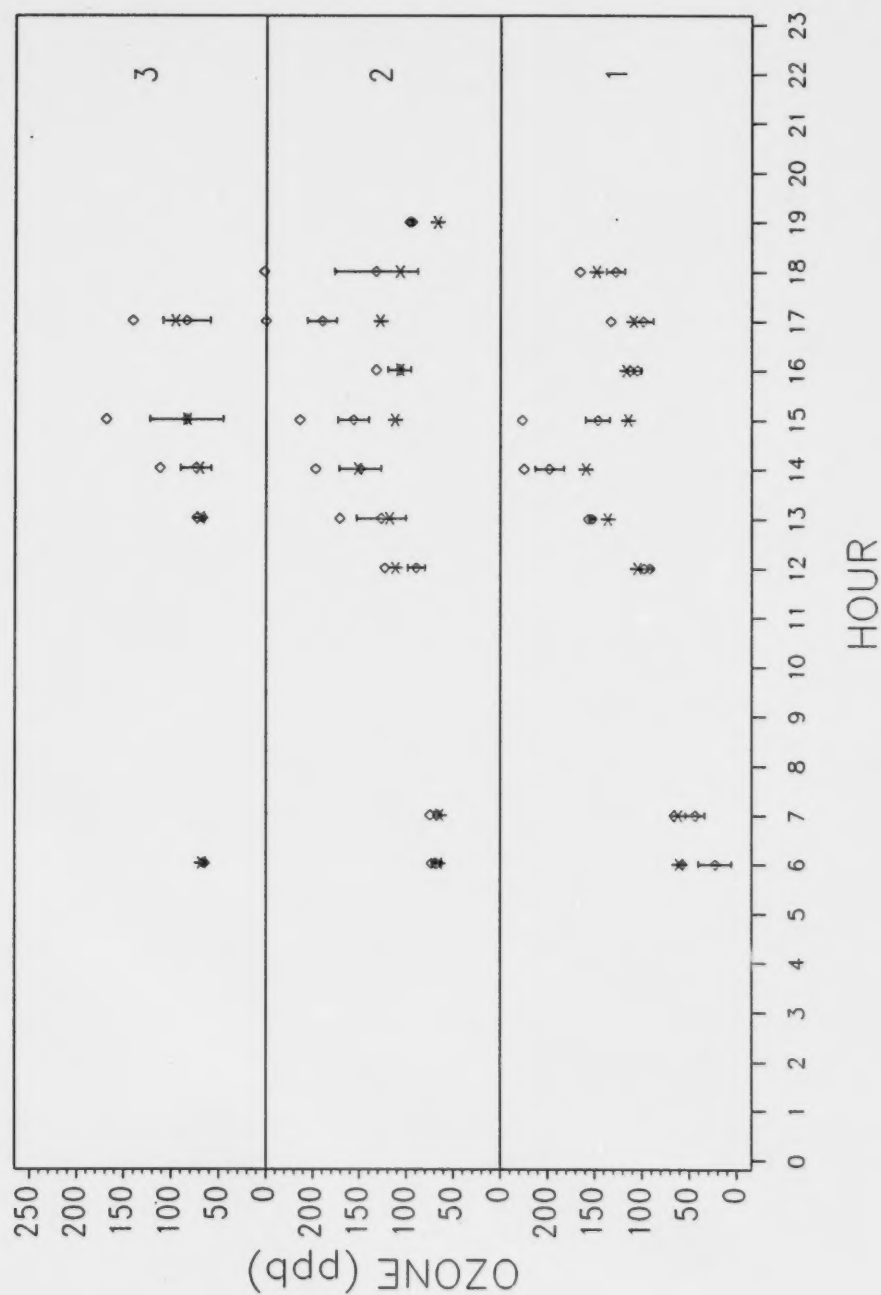


Figure 8.72. Time series of O₃ data from flight on July 22, 1980 in New York, NY area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

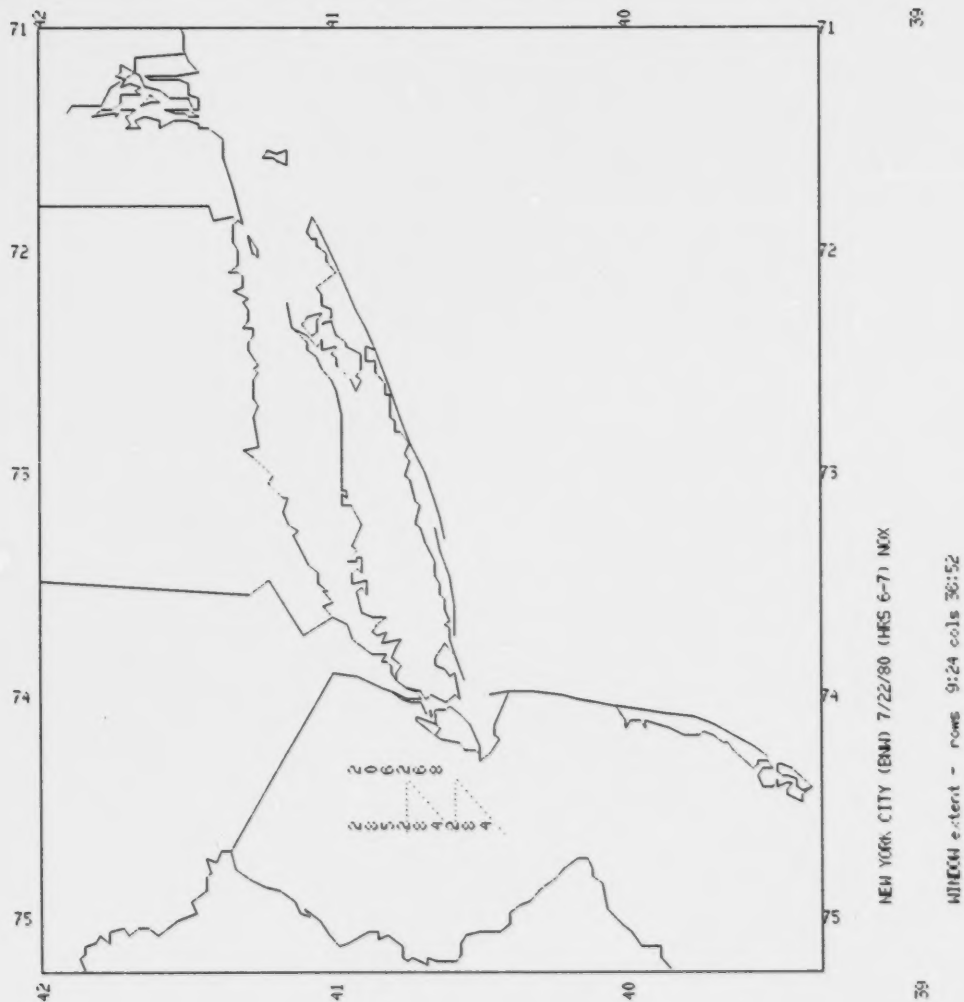


Figure 8.73. Geographical distribution of selected NO_x data from flight on July 22, 1980 in New York, NY area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

AIRCRAFT - NEW YORK CITY AREA JULY 22, 1980 (BNW)

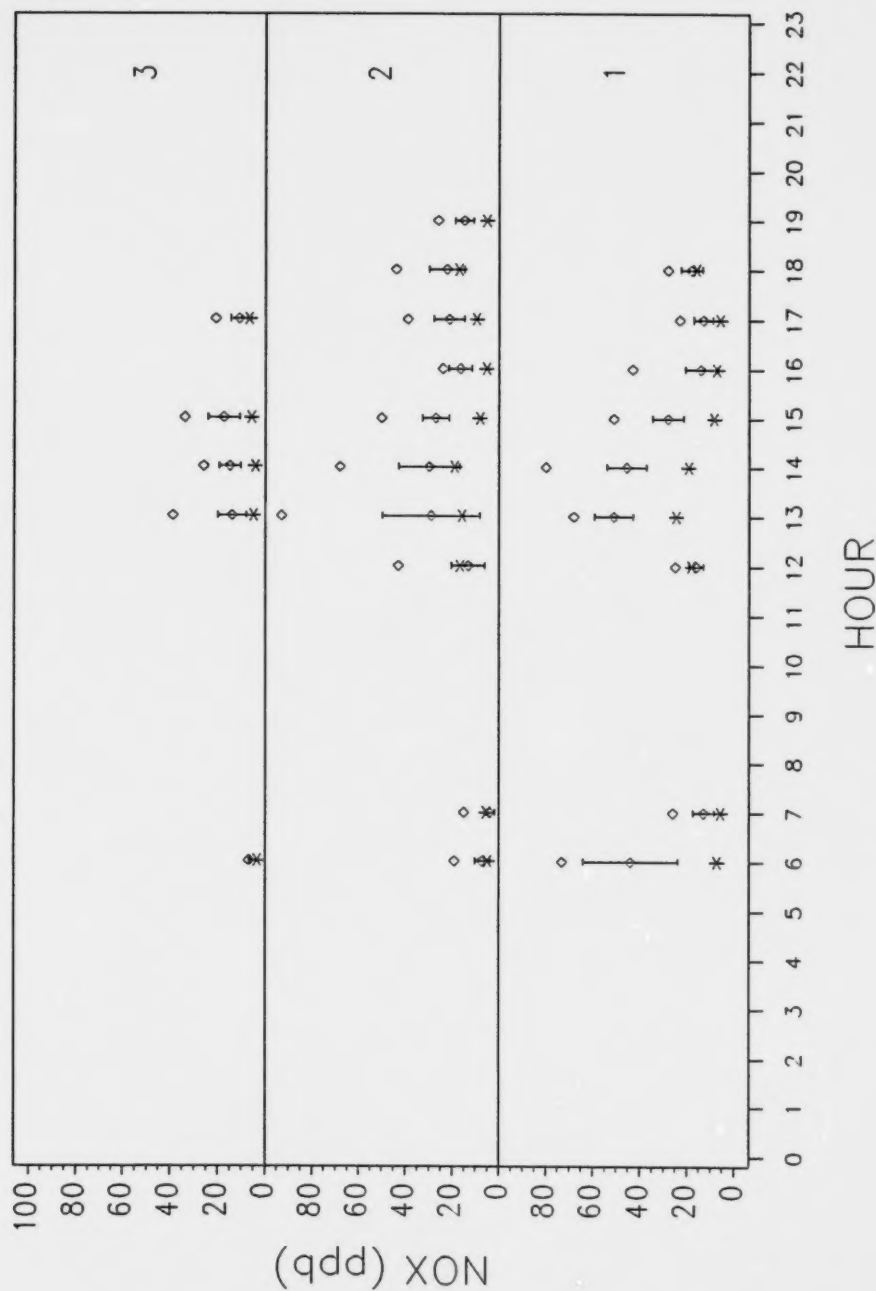


Figure 8.74. Time series of NO_x data from flight on July 22, 1980 in New York, NY area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

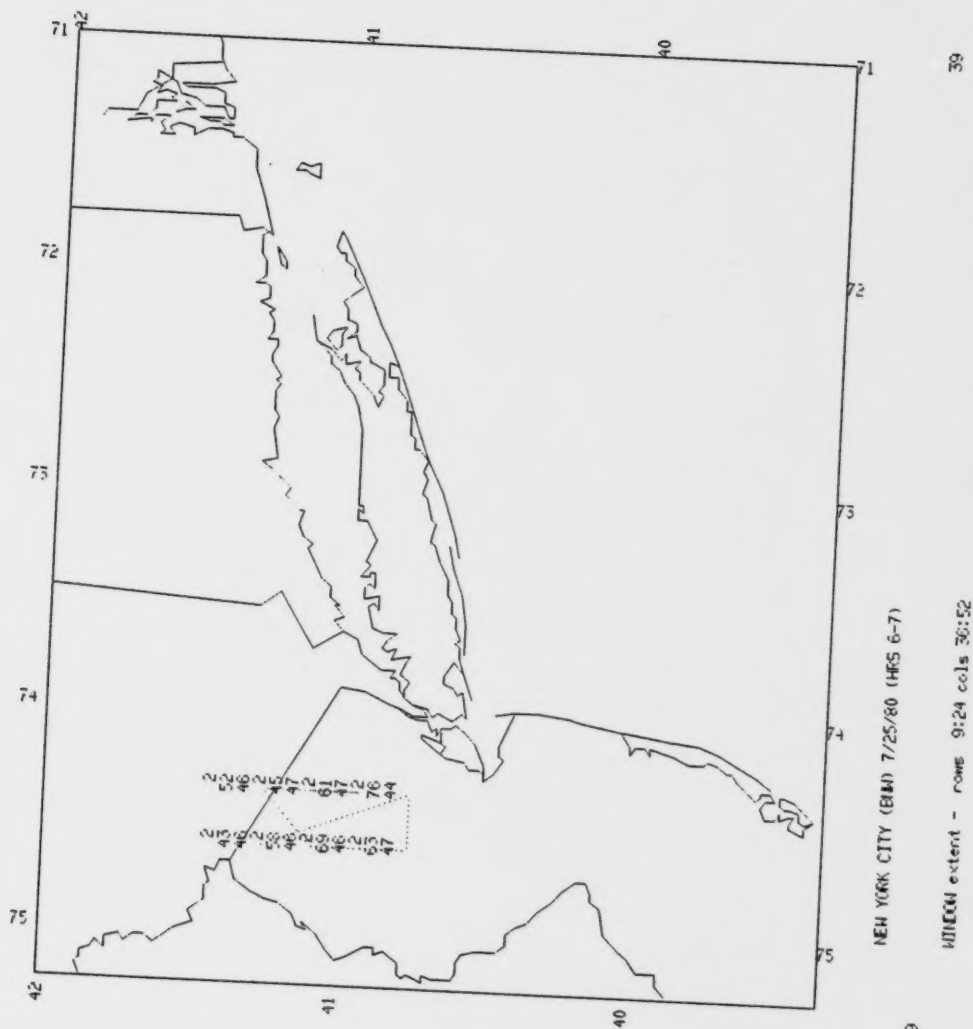
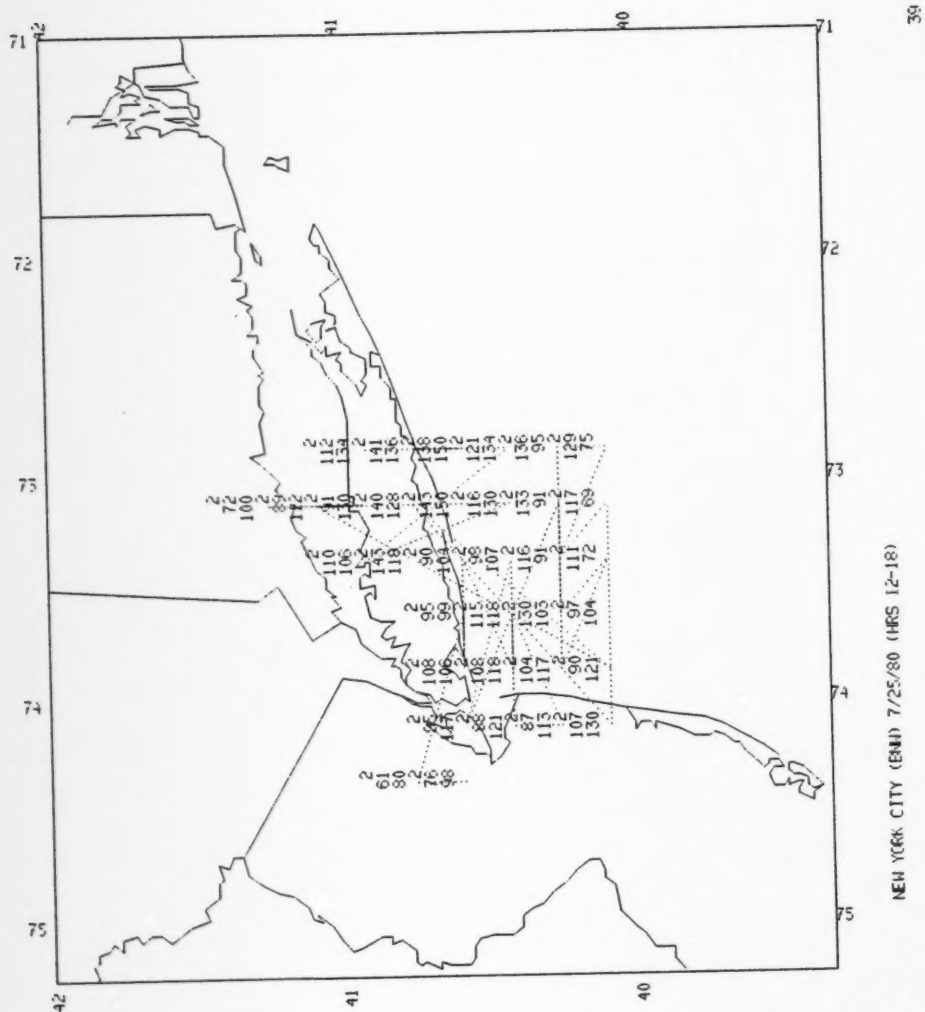


Figure 8.75. Geographical distribution of selected O₃ data from flight on July 25, 1980 in New York, NY area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).



NEW YORK CITY (BNJ) 7/25/80 (HRS 12-18)

WIND extent - rows 9:24 cols 36:52

Figure 8.75 (cont.)

AIRCRAFT - NEW YORK CITY AREA JULY 25, 1980 (BNW)

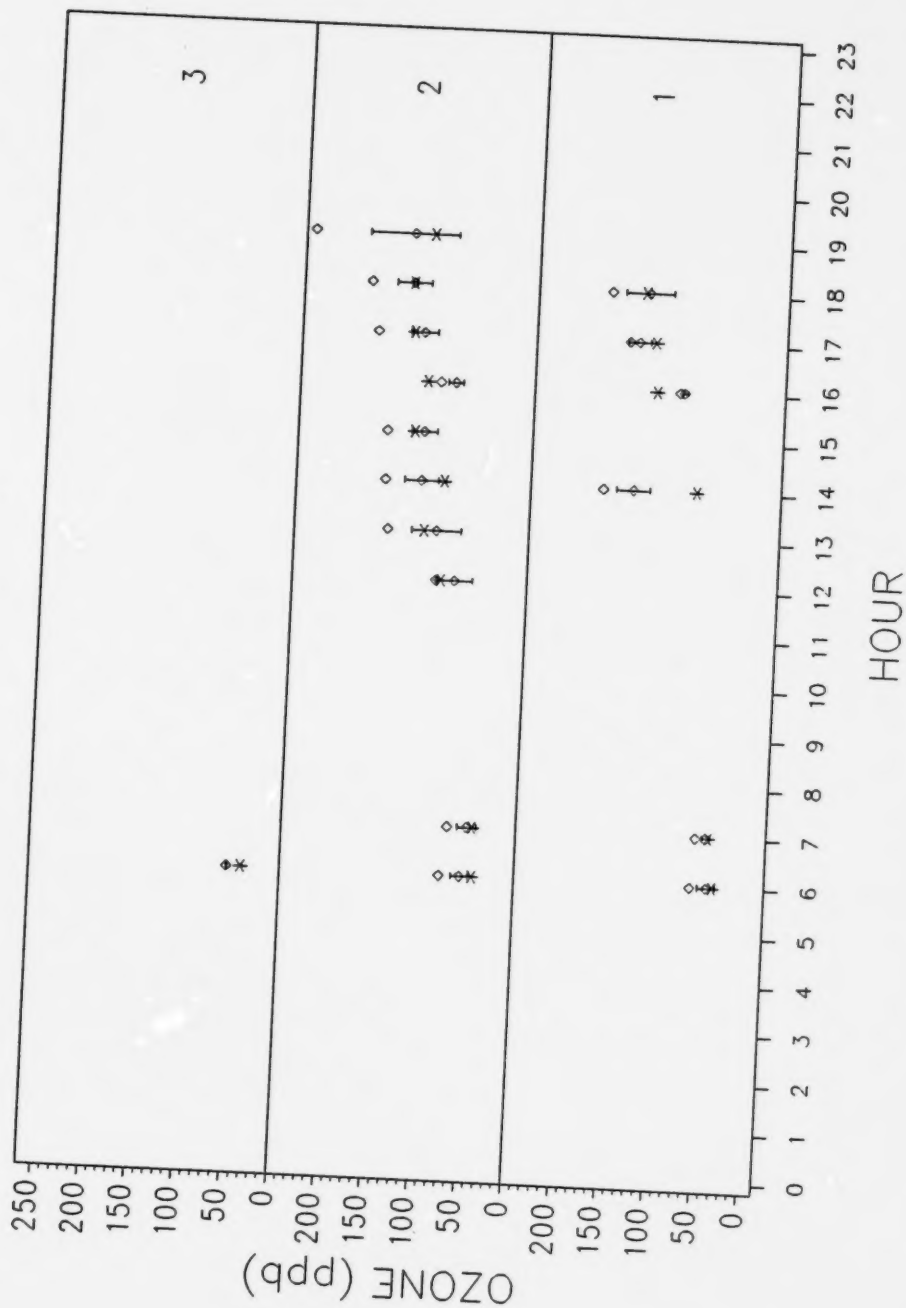


Figure 8.76. Time series of O₃ data from flight on July 25, 1980 in New York, NY area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

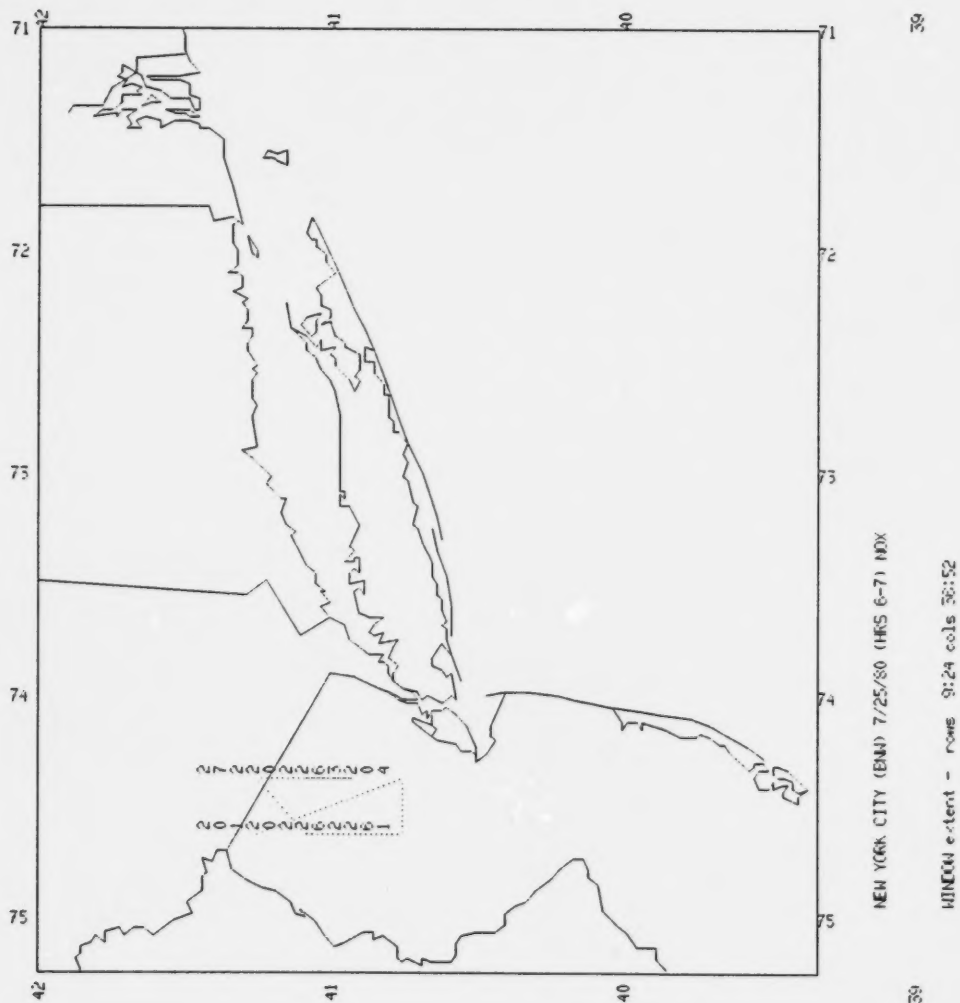
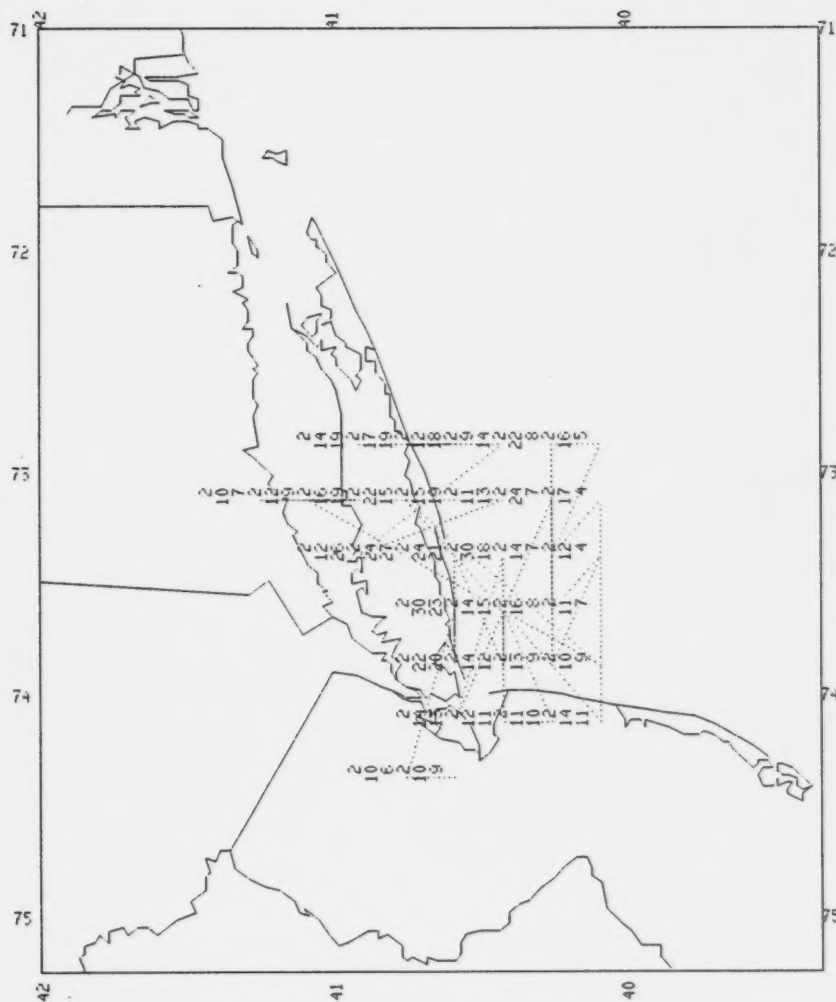


Figure 8.77. Geographical distribution of selected NO_x data from flight on July 25, 1980 in New York, NY area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).



NEW YORK CITY (BNM) 7/25/80 (HRS 12-18) MAX

WIND extent - none 9:24 cols 30:52

Figure 8.77 (cont.)

AIRCRAFT - NEW YORK CITY AREA JULY 25, 1980 (BNW)

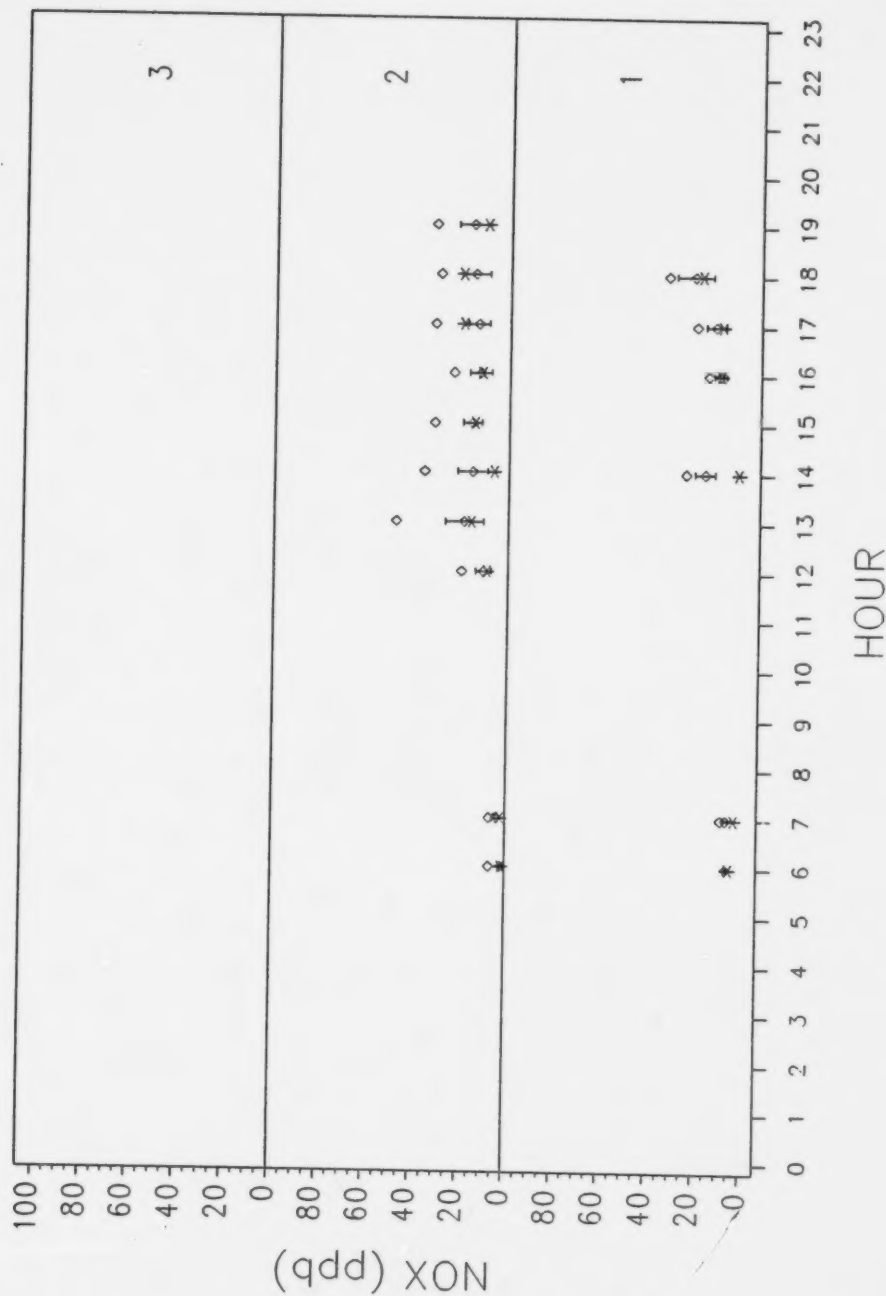


Figure 8.78. Time series of NO_x data from flight on July 25, 1980 in New York, NY area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

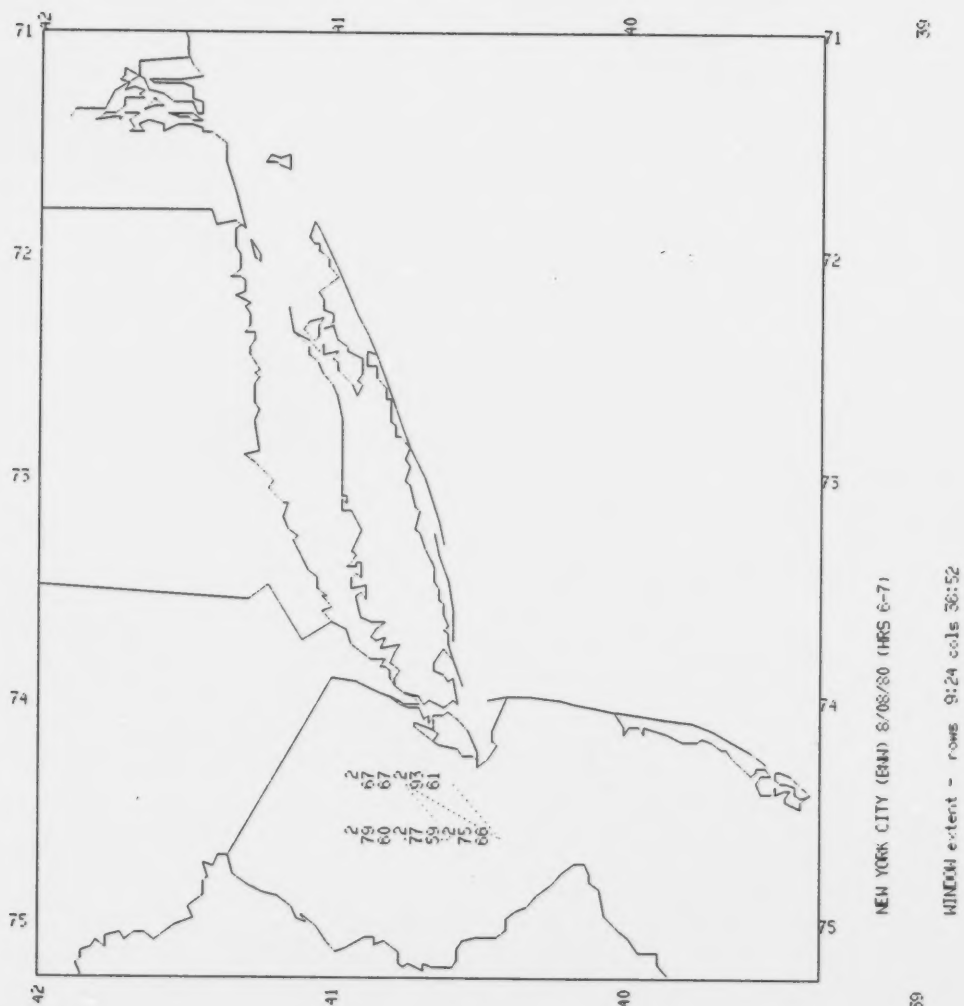
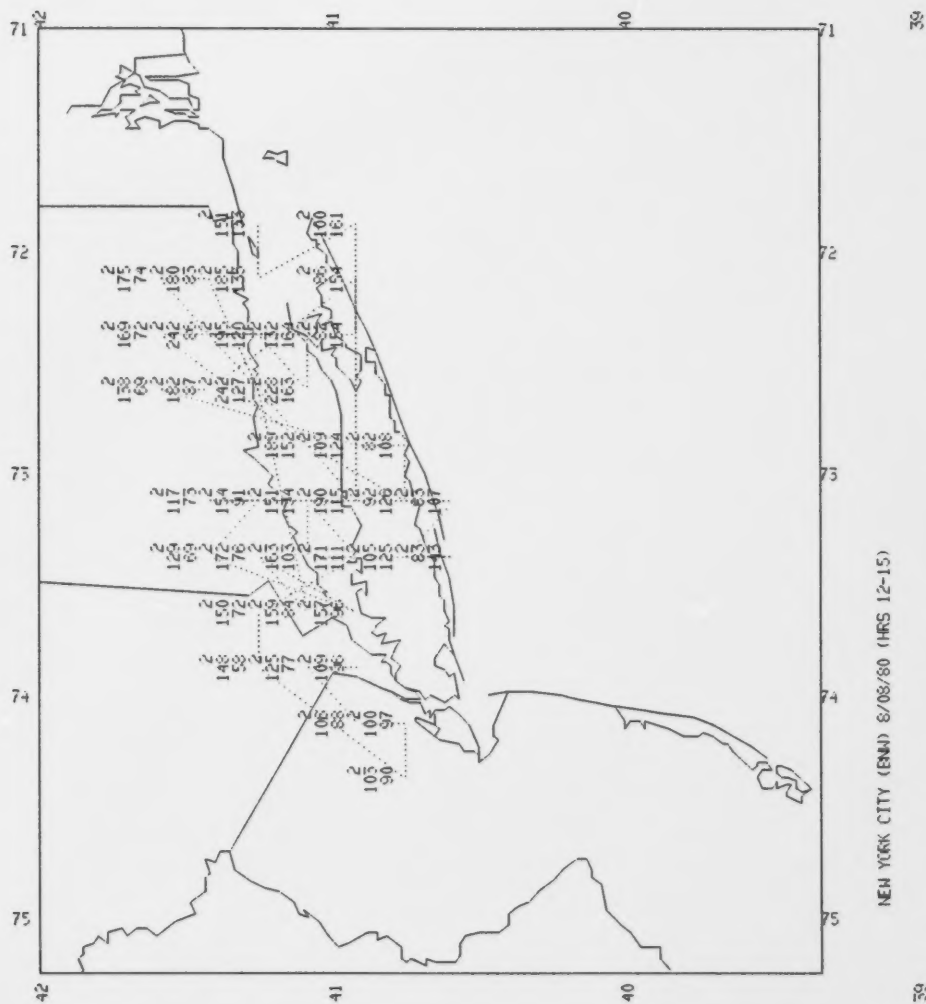


Figure 8.79. Geographical distribution of selected O_3 data from flight on Aug. 8, 1980 in New York, NY area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).



AIRCRAFT - NEW YORK CITY AREA AUGUST 8, 1980 (BNW)

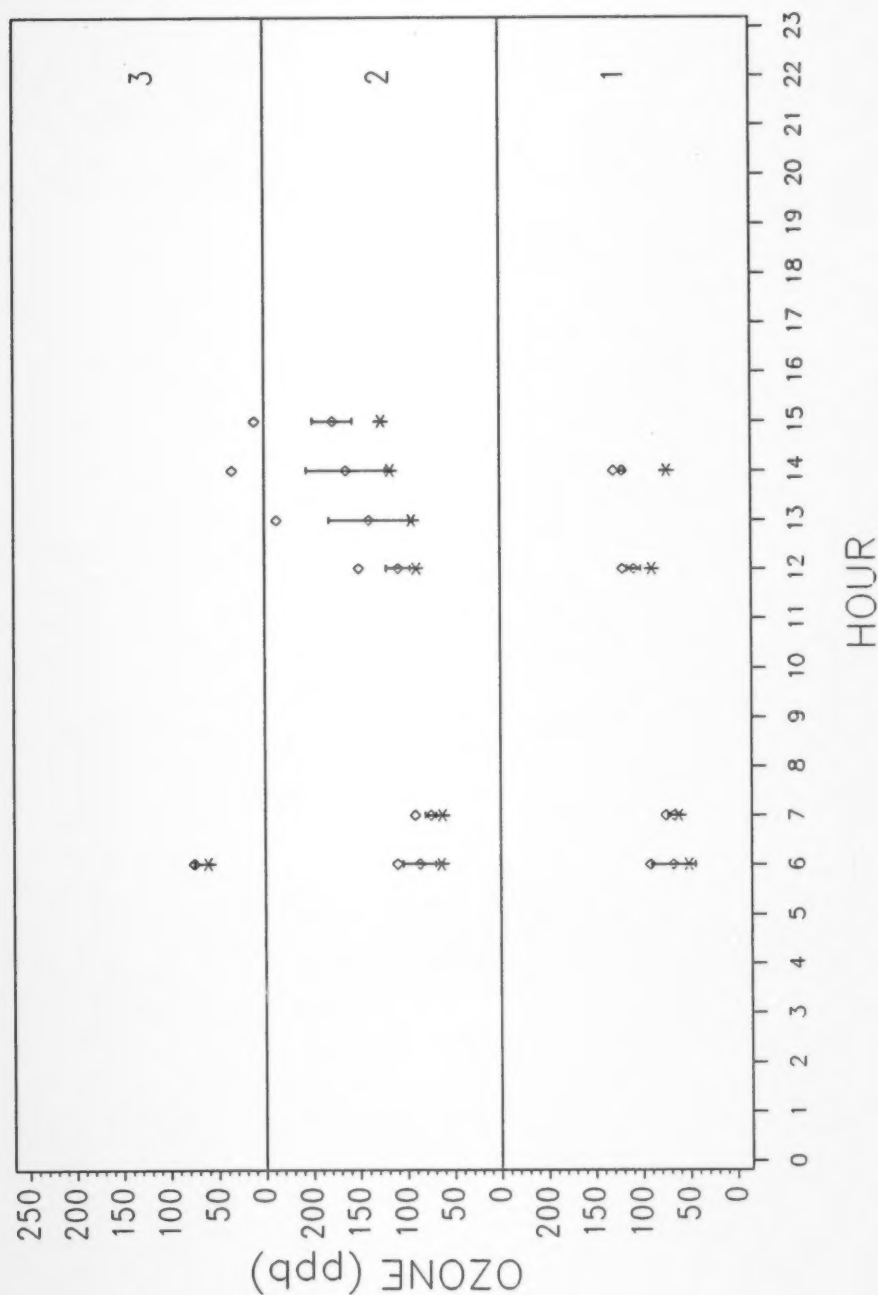


Figure 8.80. Time series of O₃ data from flight on Aug. 8, 1980 in New York, NY area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

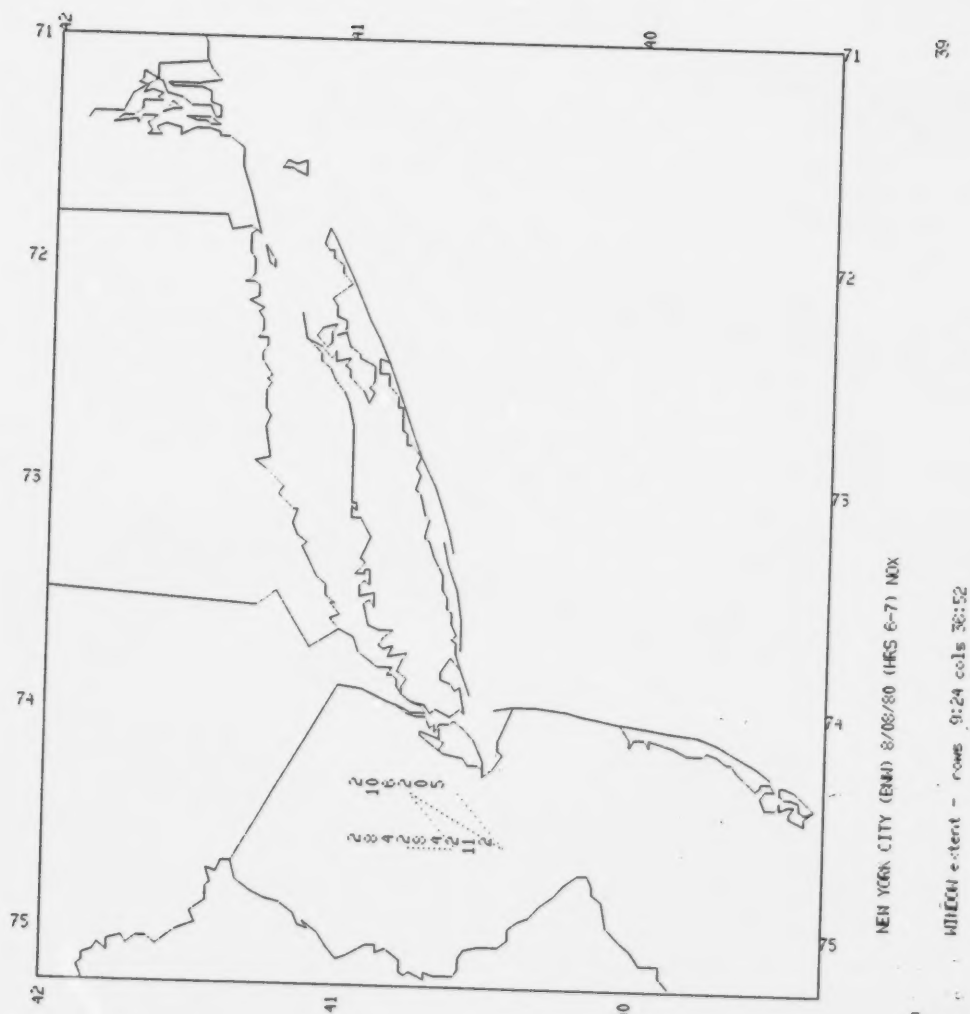


Figure 8.81. Geographical distribution of selected NO_x data from flight on Aug. 8, 1980 in New York, NY area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

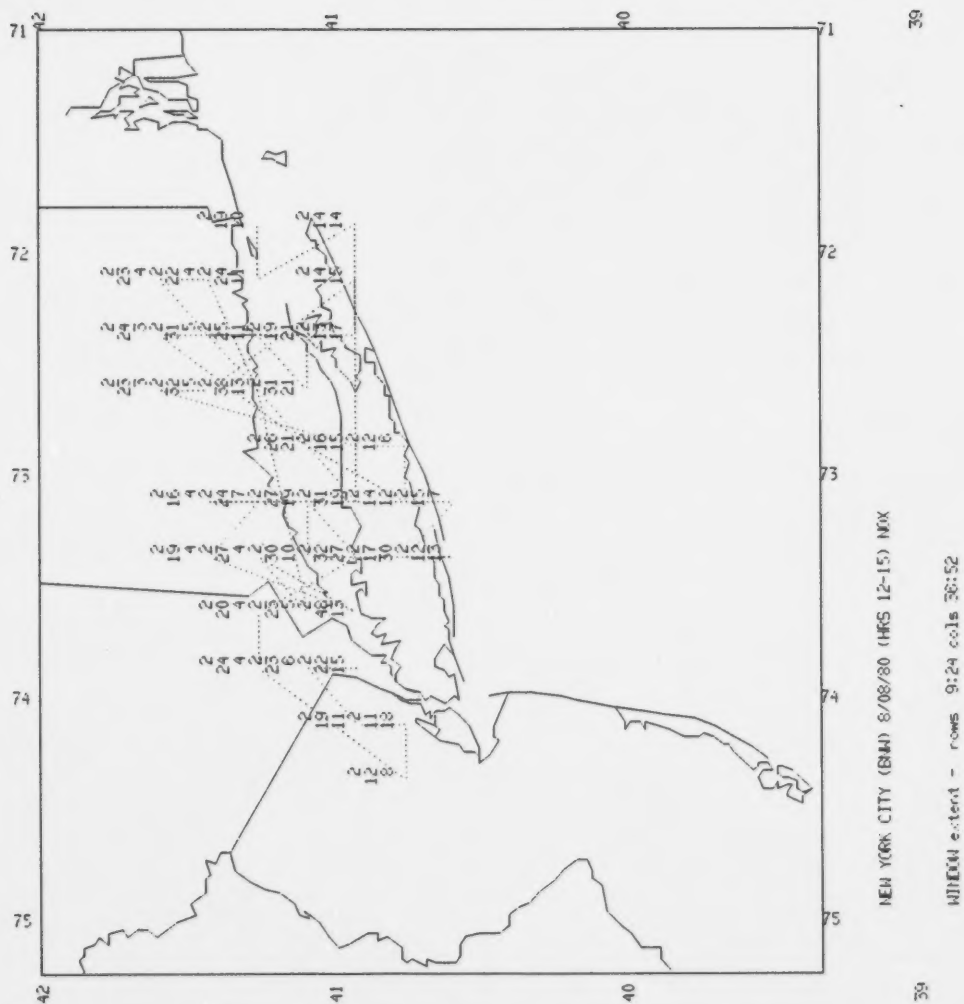


Figure 8.81 (cont.)

AIRCRAFT - NEW YORK CITY AREA AUGUST 8, 1980 (BNW)

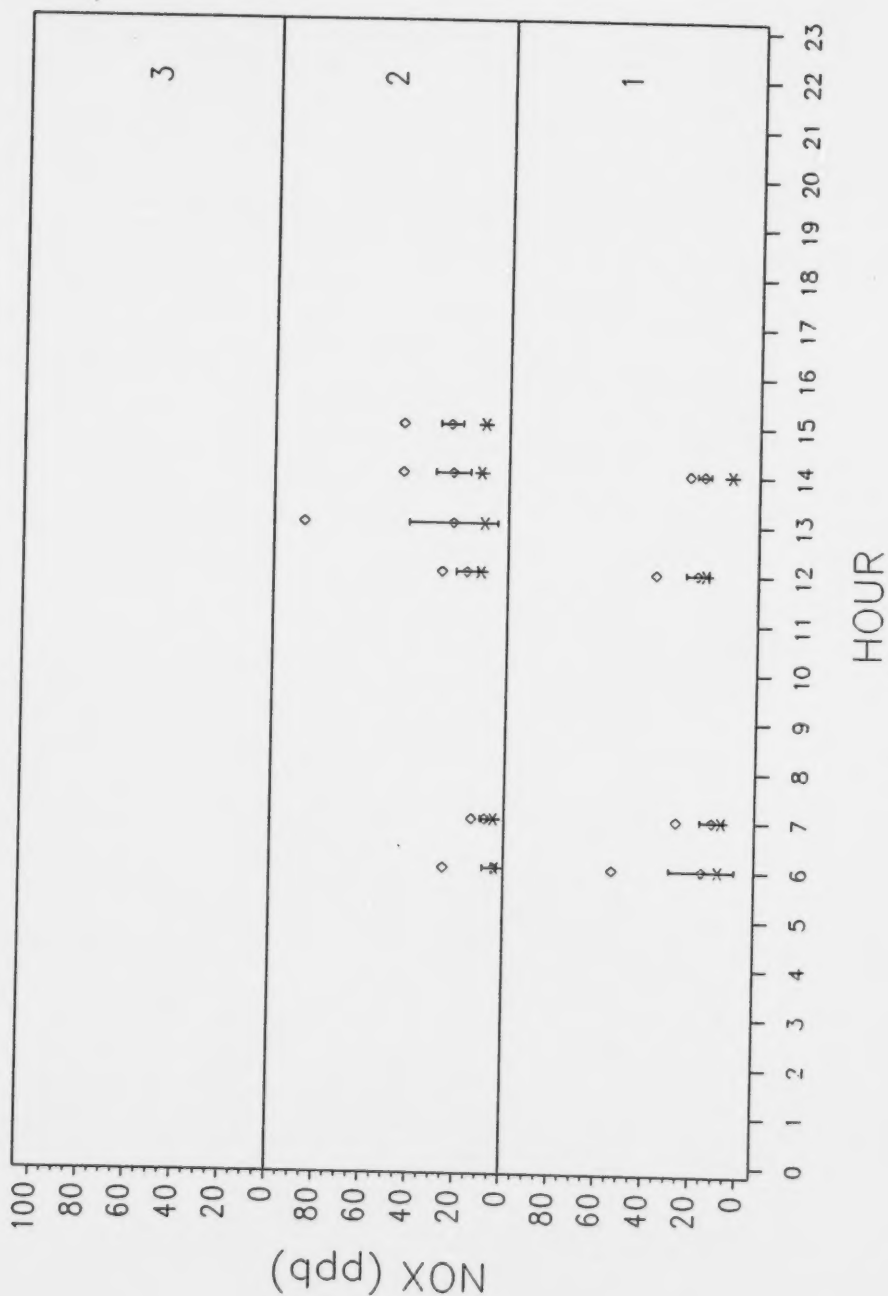
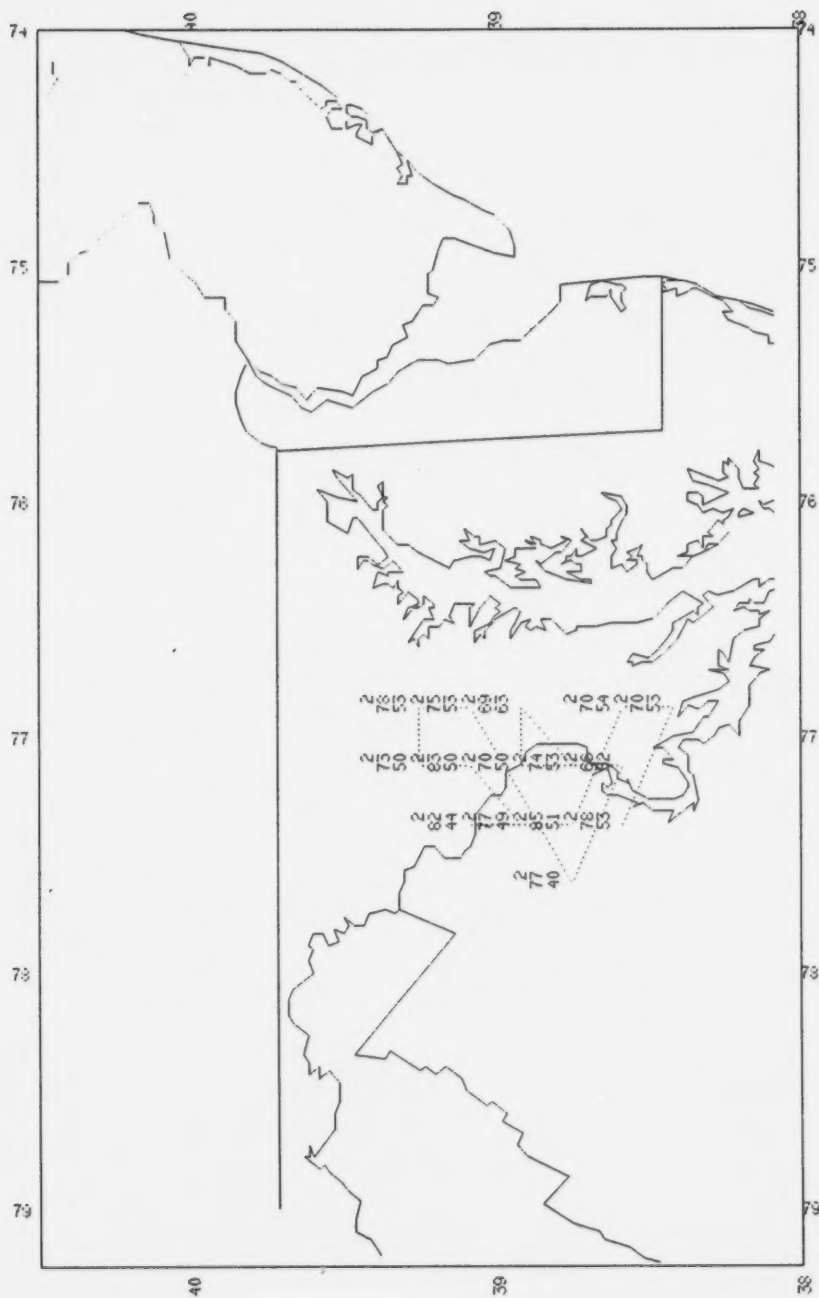


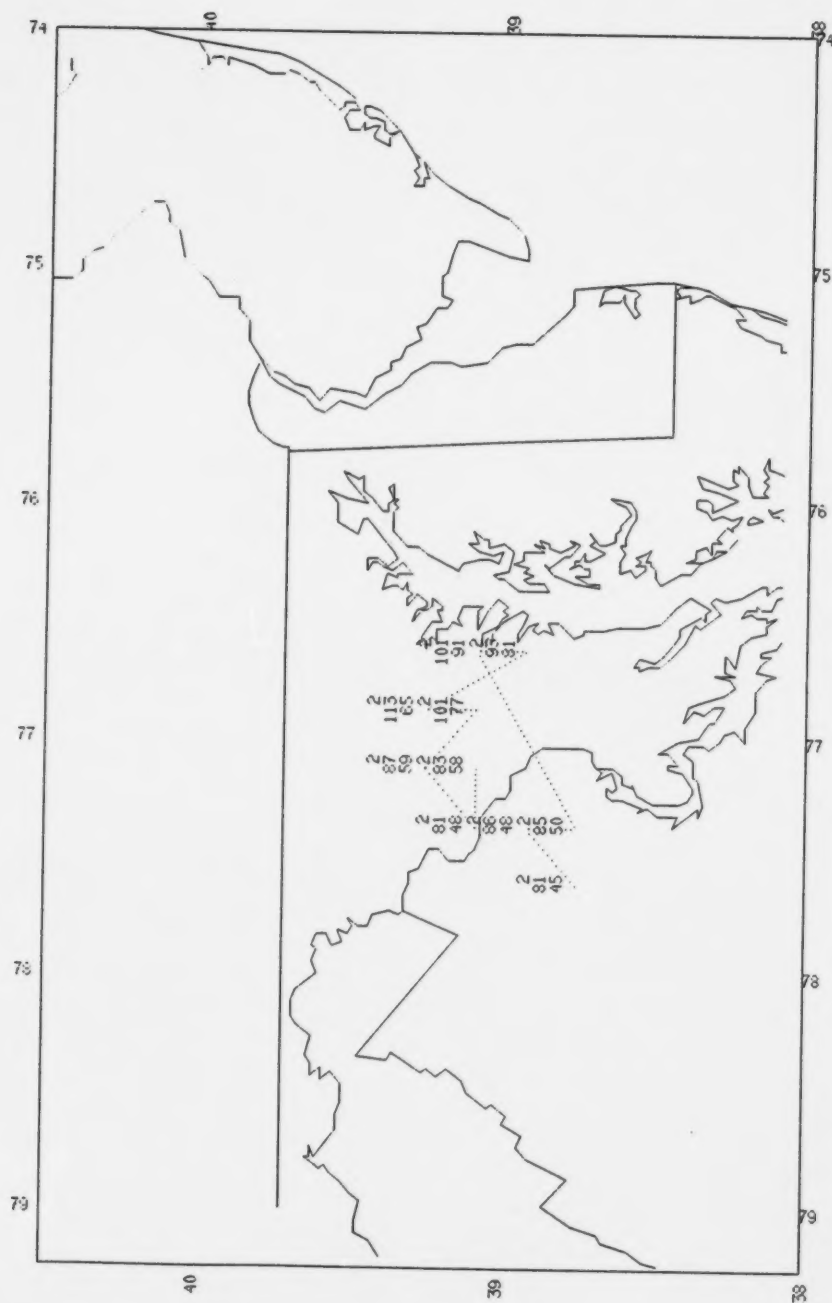
Figure 8.82. Time series of NO_x data from flight on Aug. 8, 1980 in New York, NY area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.



WASHINGTON, D.C. (EPA) 7/15/80 (HRS 5-10)

WINDW e-tent - rows 1:15 cols 20:40

Figure 8.83. Geographical distribution of selected O₃ data from flight on July 15, 1980 in Washington, DC area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).



WASHINGTON, D.C. (EPA) 7/15/80 (HRS 13-16)

WINDOW extent - rows 1:15 cols 20:40

Figure 8.83 (cont.)

AIRCRAFT — WASHINGTON, D.C. AREA JULY 15, 1980 (EPA)

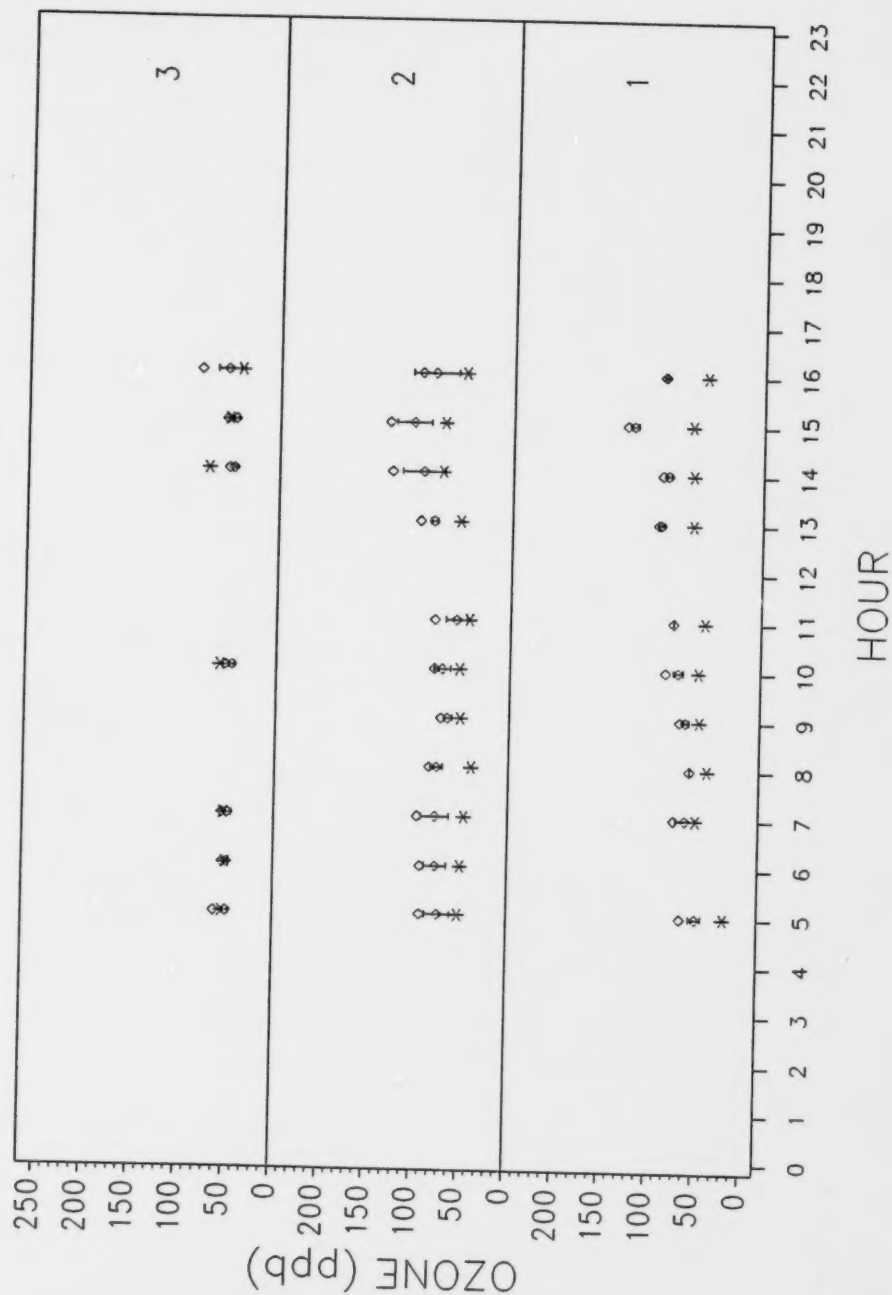


Figure 8.84. Time series of O₃ data from flight on July 15, 1980 in Washington, DC area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

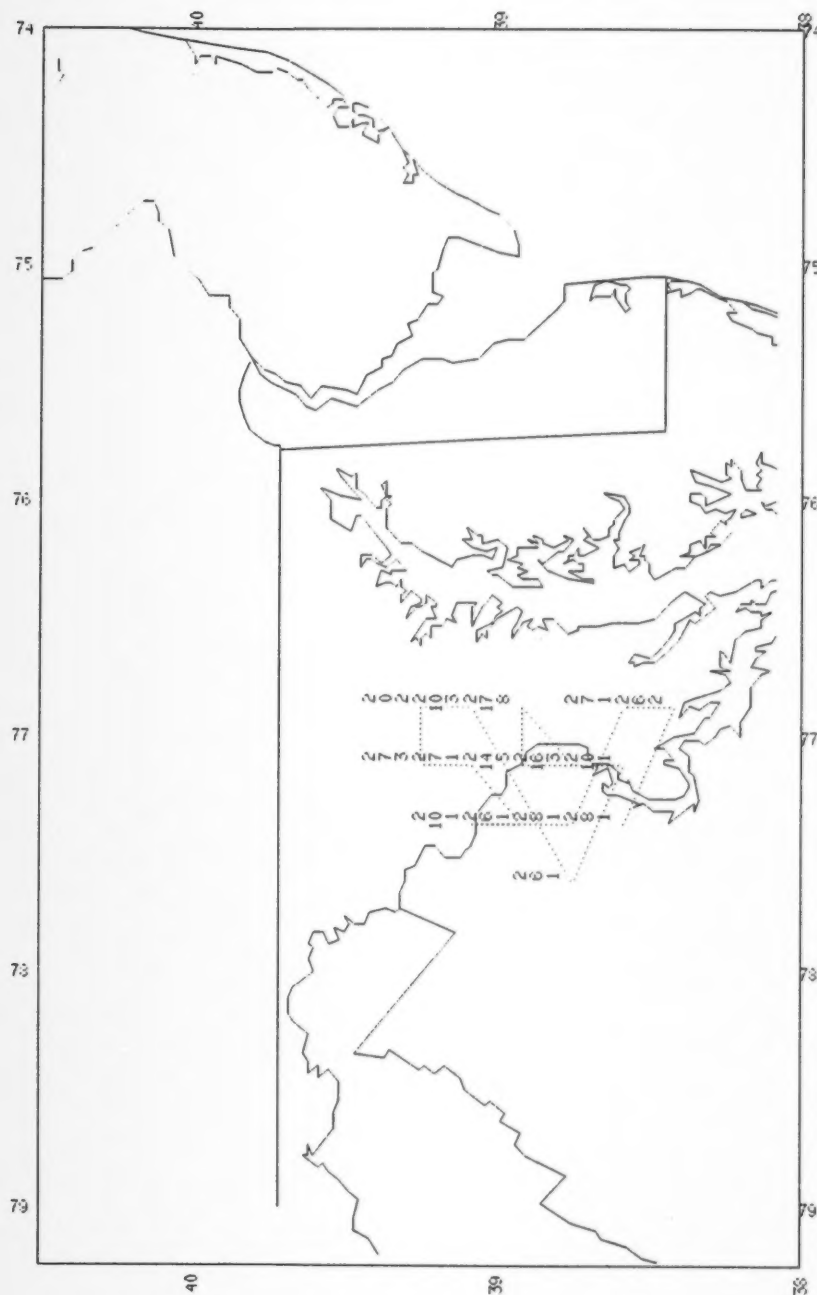


Figure 8.85. Geographical distribution of selected NO_x data from flight on July 15, 1980 in Washington, DC area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

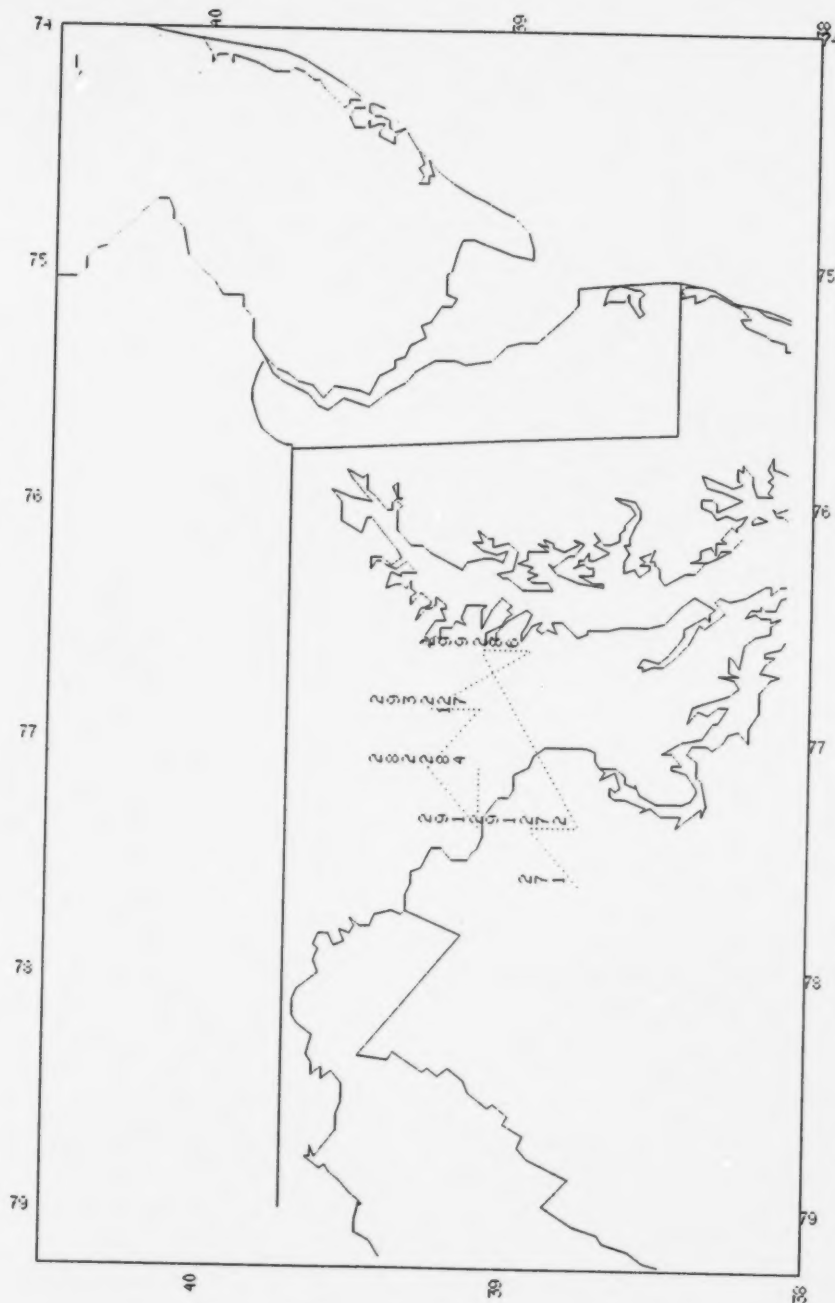


Figure 8.85 (cont.)

AIRCRAFT - WASHINGTON, D.C. AREA
JULY 15, 1980 (EPA)

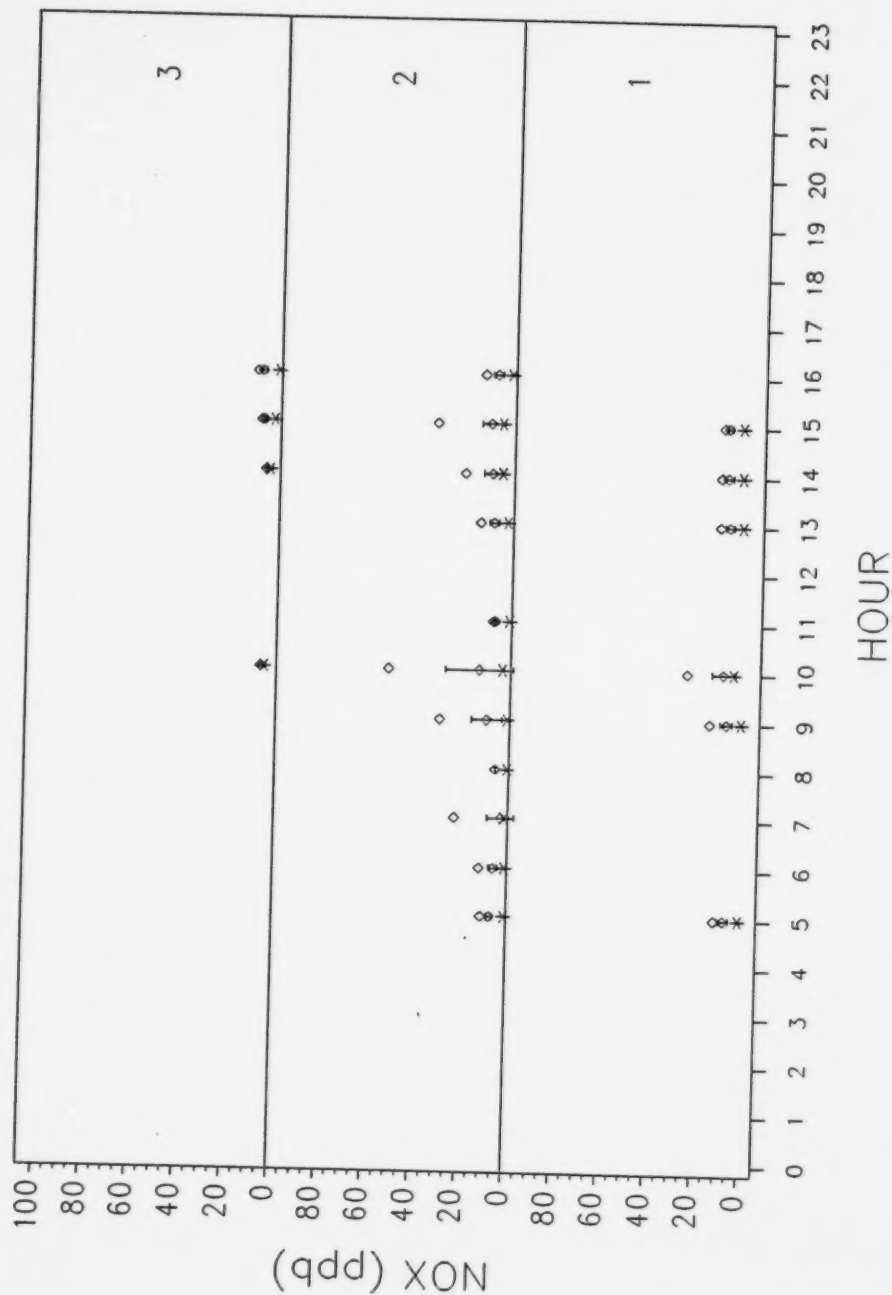
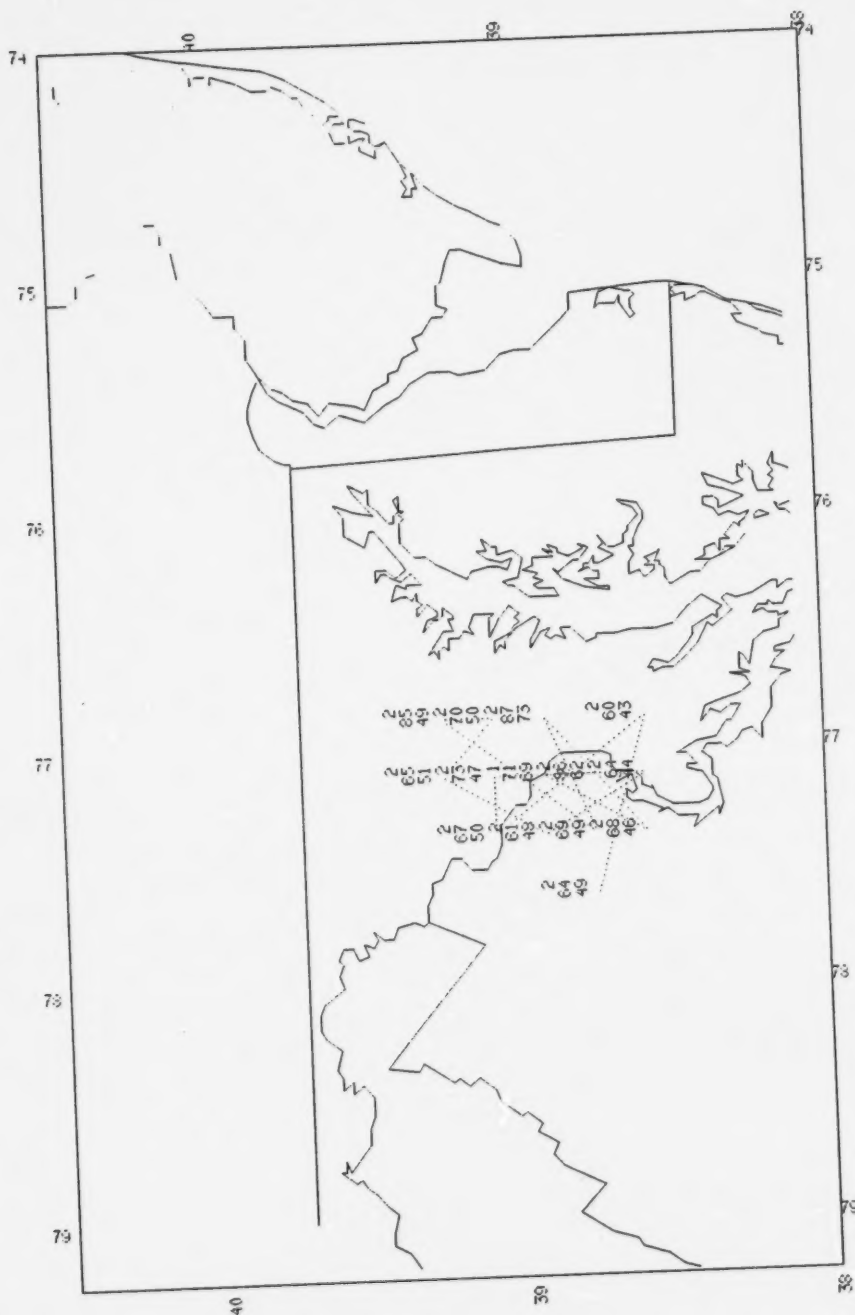


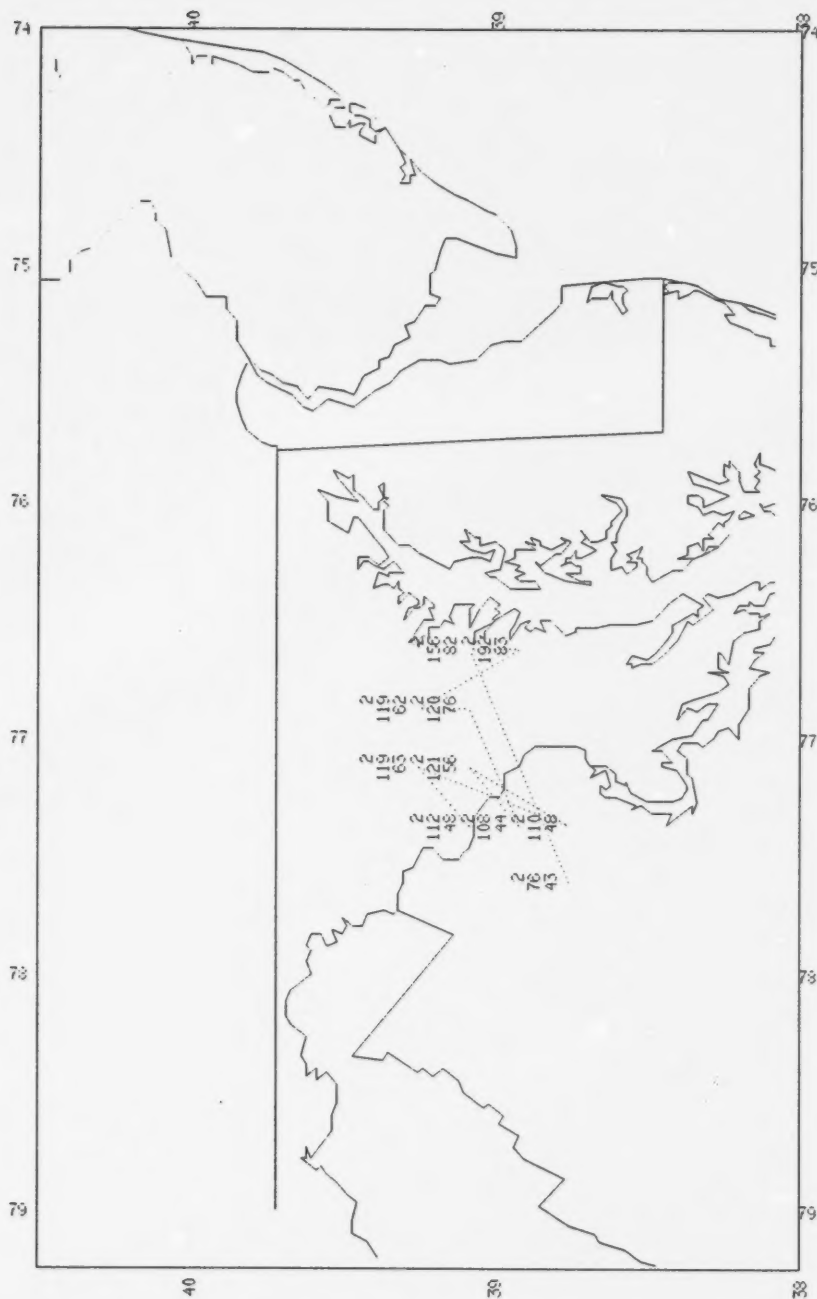
Figure 8.86. Time series of NO_x data from flight on July 15, 1980 in Washington, DC area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.



WASHINGTON, D.C. (EPA) 7/21/80 (HFS 5-10)

WINDON extent - rows 1:15 cols 20:40

Figure 8.87. Geographical distribution of selected O₃ data from flight on July 21, 1980 in Washington, DC area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).



WASHINGTON, D.C. (EPA) 7/21/80 (HRS 13-15)

MINIMUM extent - rows 1:15 cols 20:40

Figure 8.87 (cont.)

AIRCRAFT - WASHINGTON, D.C. AREA JULY 21, 1980 (EPA)

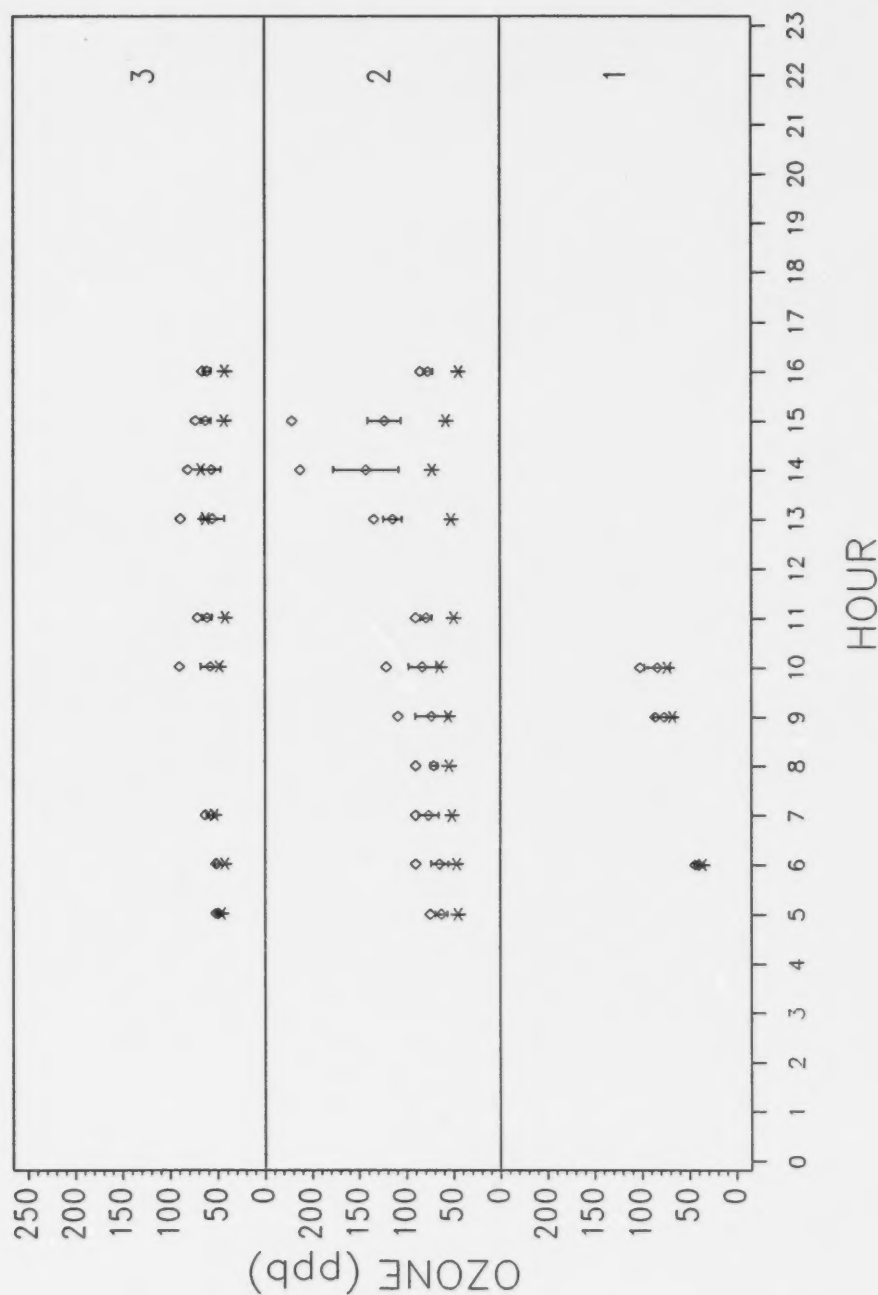


Figure 8.88. Time series of O₃ data from flight on July 21, 1980 in Washington, DC area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

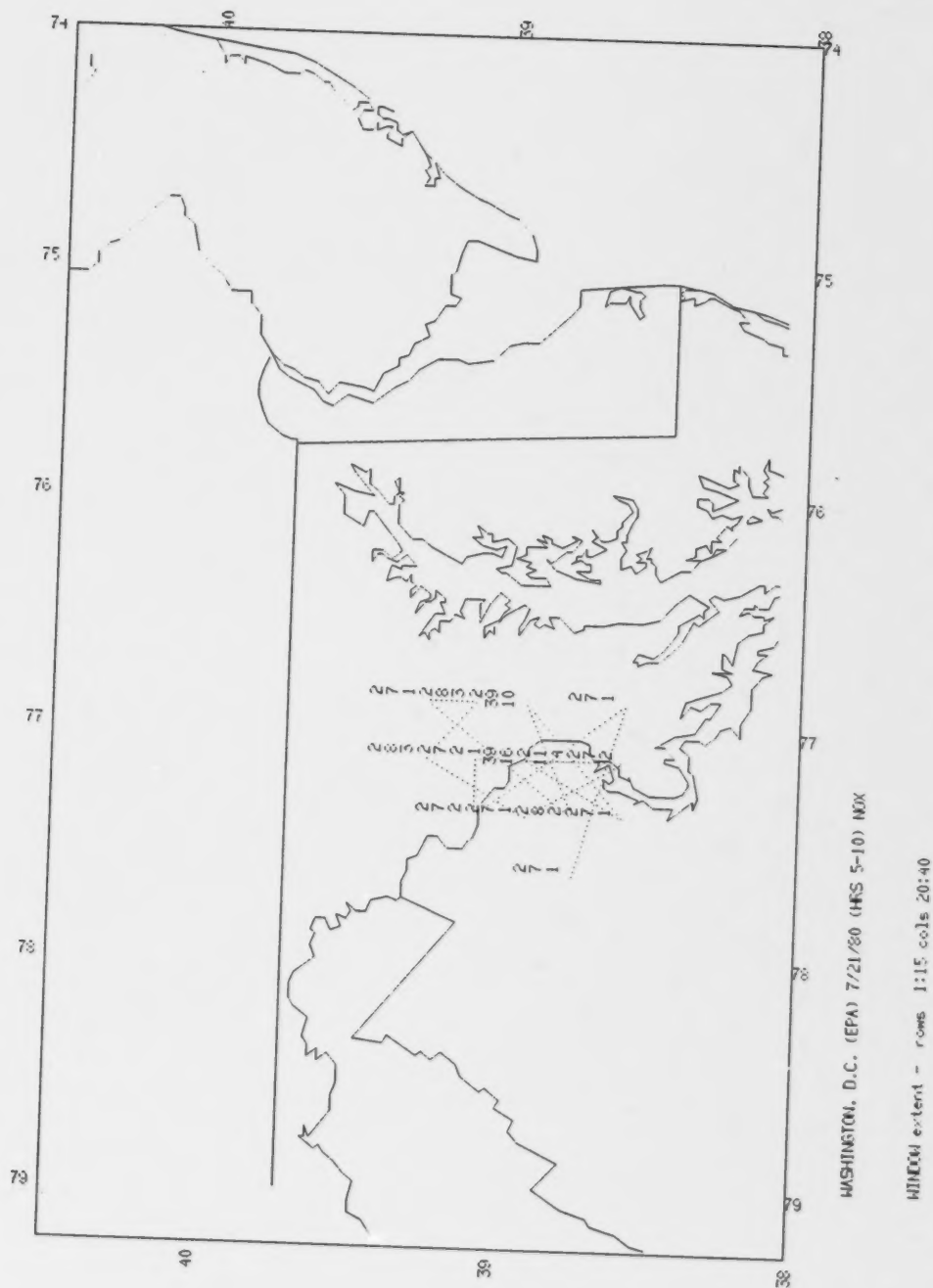
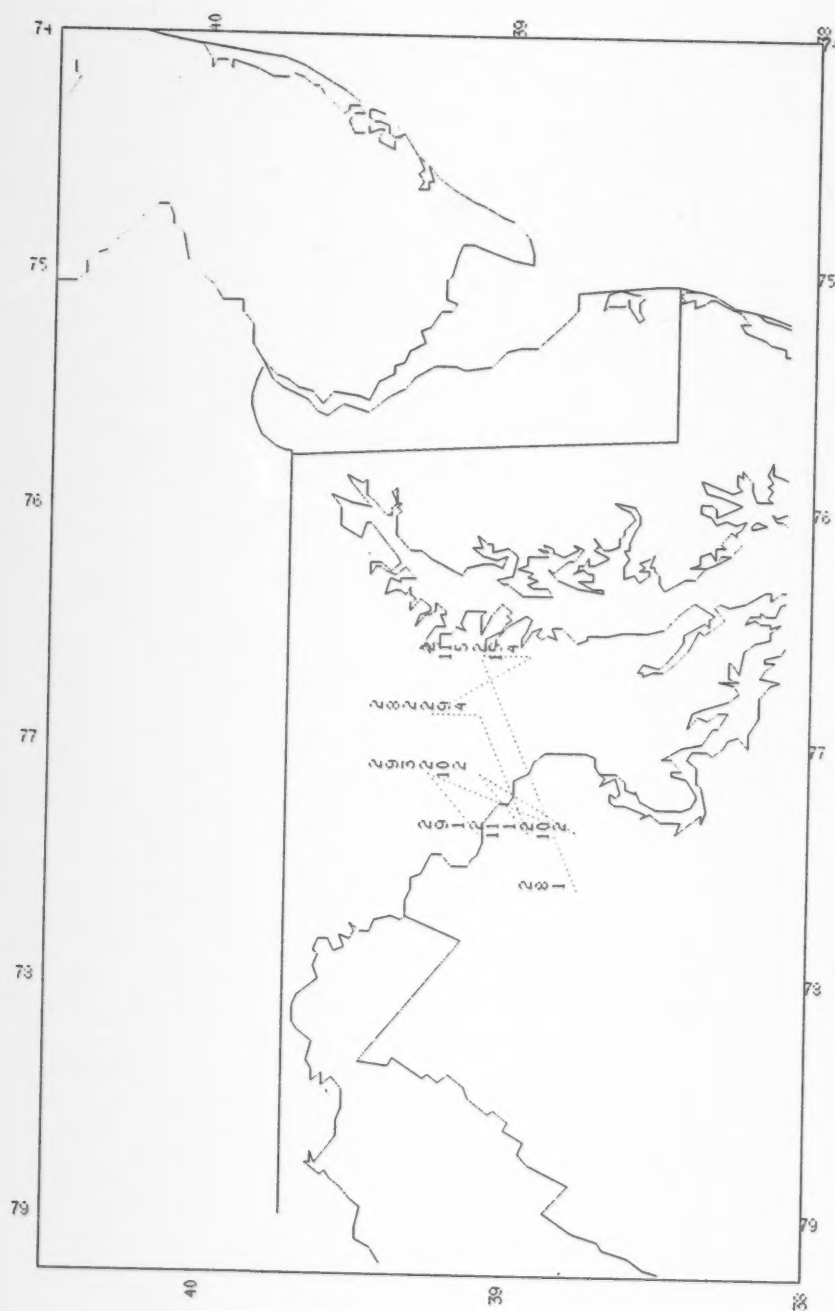


Figure 8.89. Geographical distribution of selected NO_x data from flight on July 21, 1980 in Washington, DC area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).



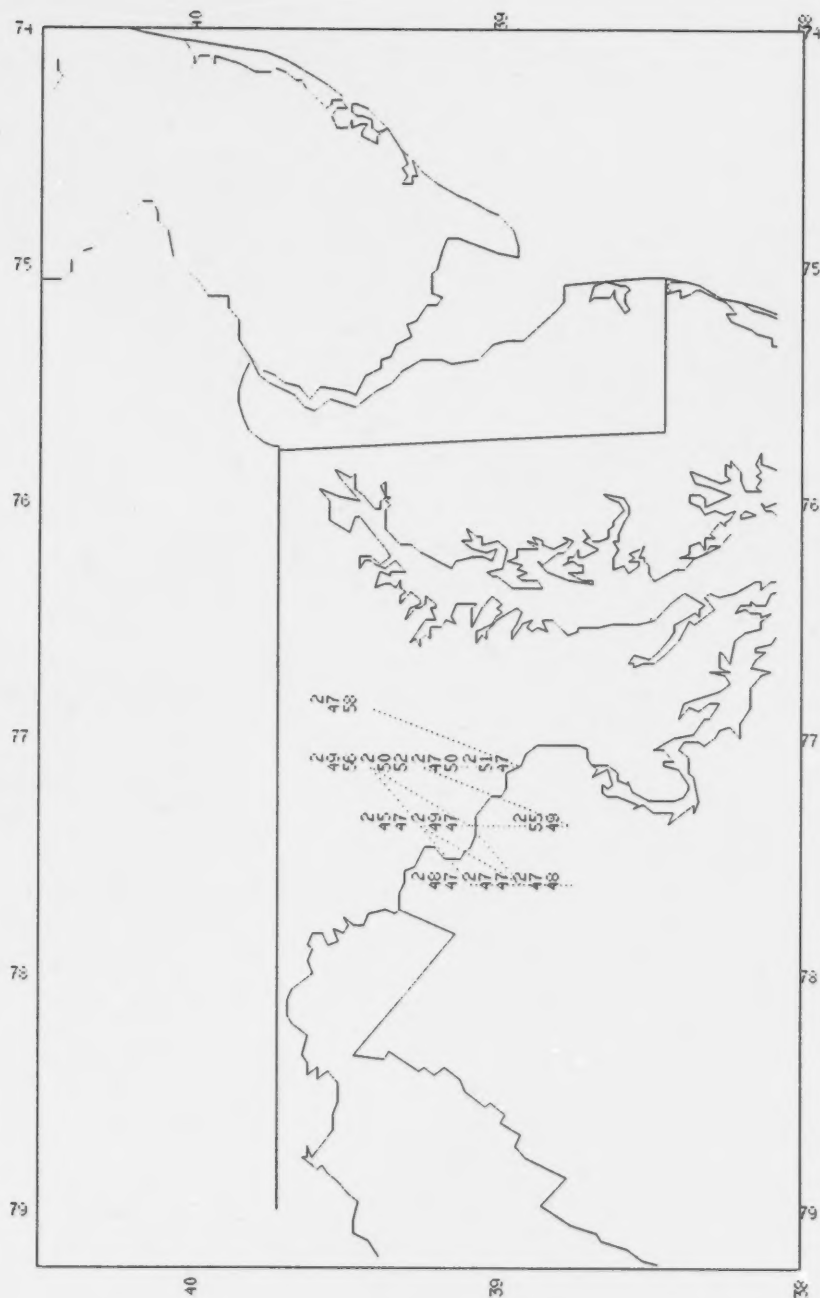
HTML extent - rows 1:15 cols 20:40

Figure 8.89 (cont.)

AIRCRAFT — WASHINGTON, D.C. AREA
JULY 21, 1980 (EPA)



Figure 8.90. Time series of NO_x data from flight on July 21, 1980 in Washington, DC area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.



WASHINGTON, D.C. (EPA) 7/25/80 (HKS 4-6)

WINDON extent - rows 1:15 cols 20:40

Figure 8.91. Geographical distribution of selected O₃ data from flight on July 25, 1980 in Washington, DC area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).

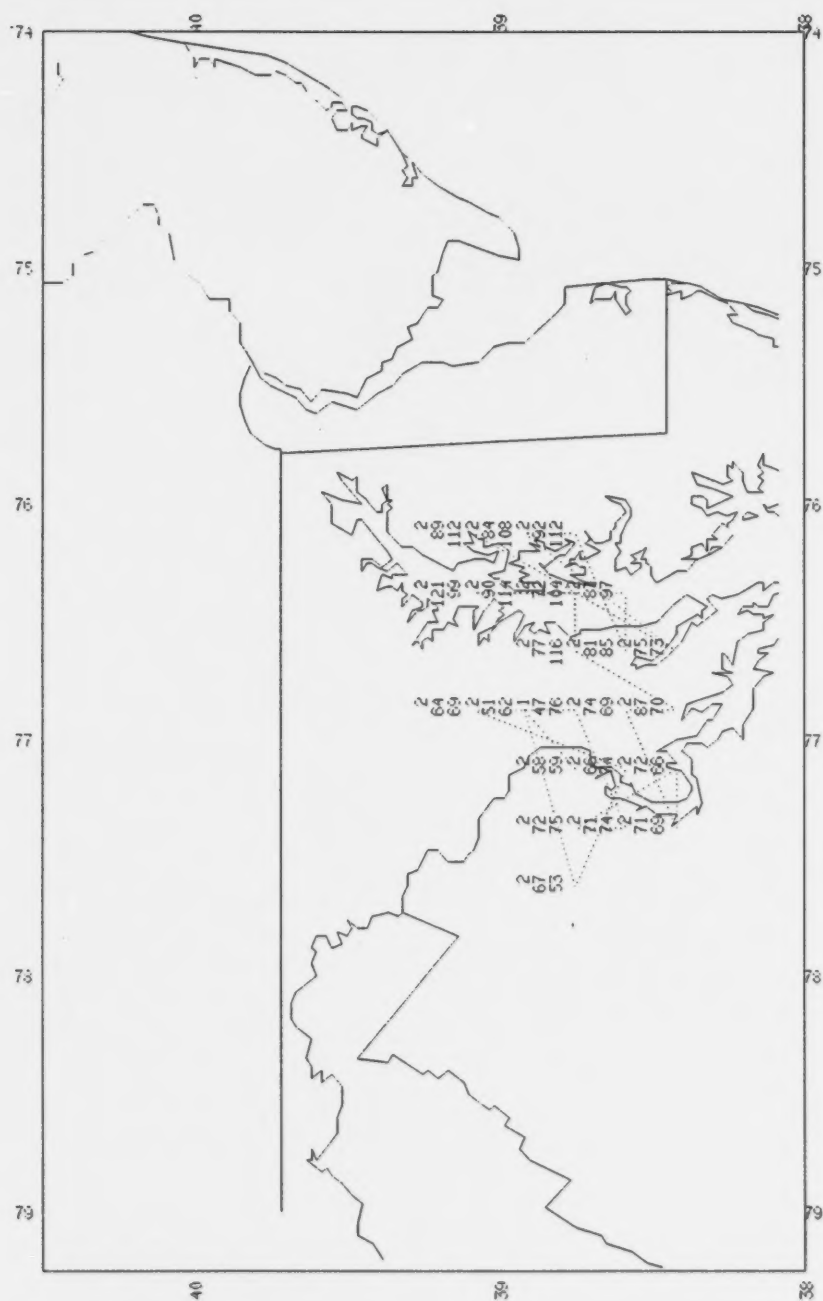


Figure 8.91 (cont.)

AIRCRAFT - WASHINGTON, D.C. AREA JULY 25, 1980 (EPA)

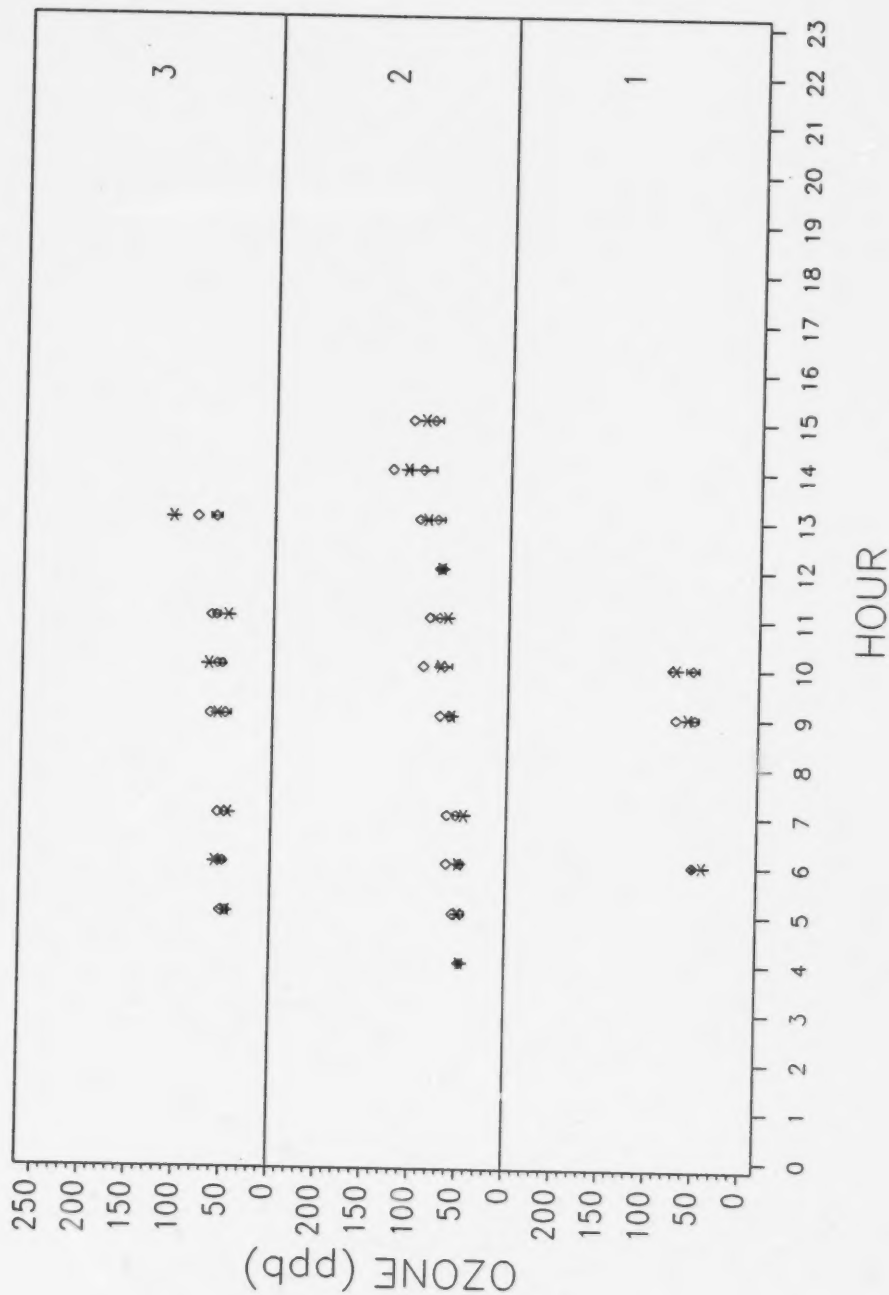


Figure 8.92. Time series of O₃ data from flight on July 25, 1980 in Washington, DC area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

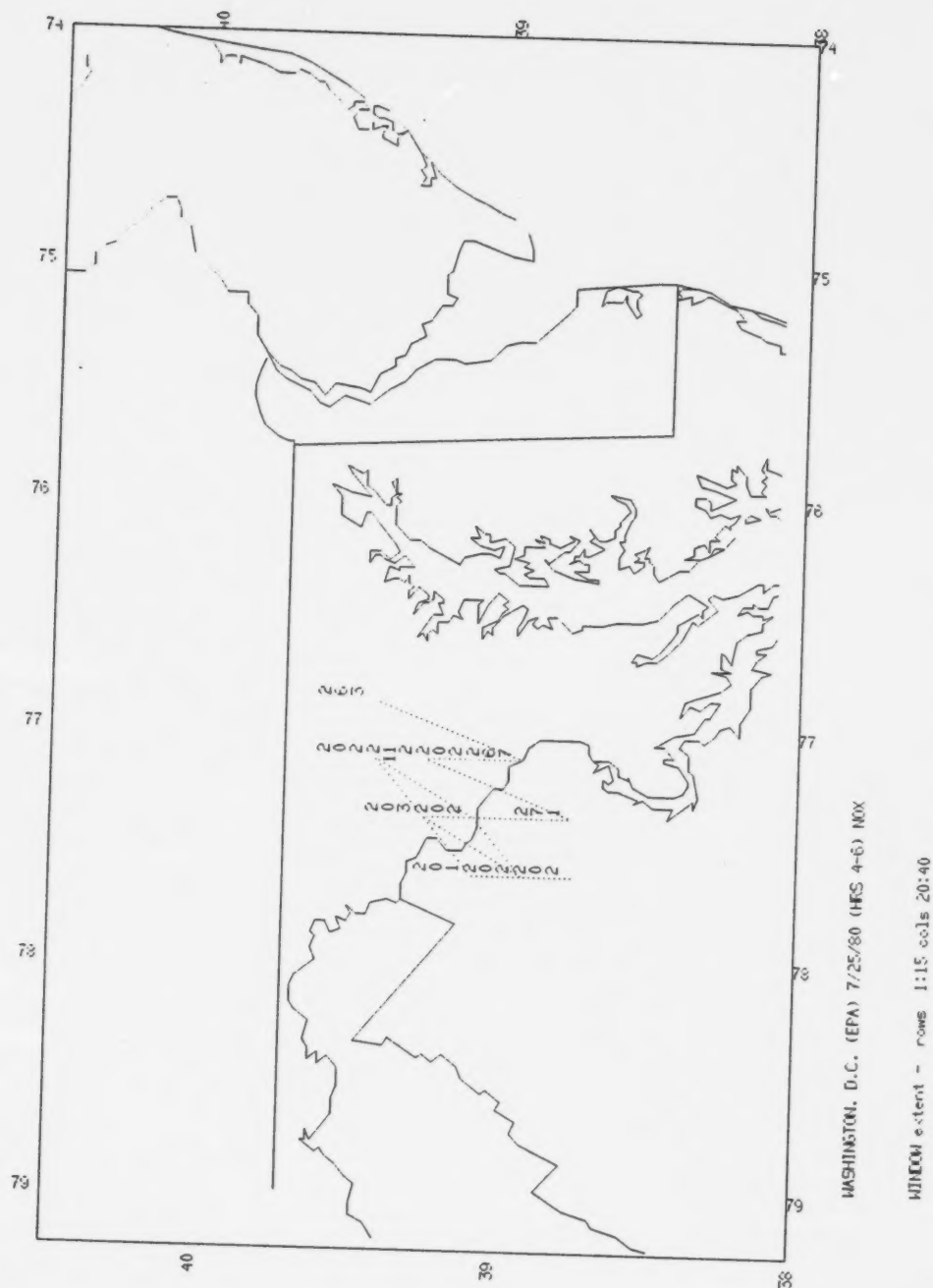
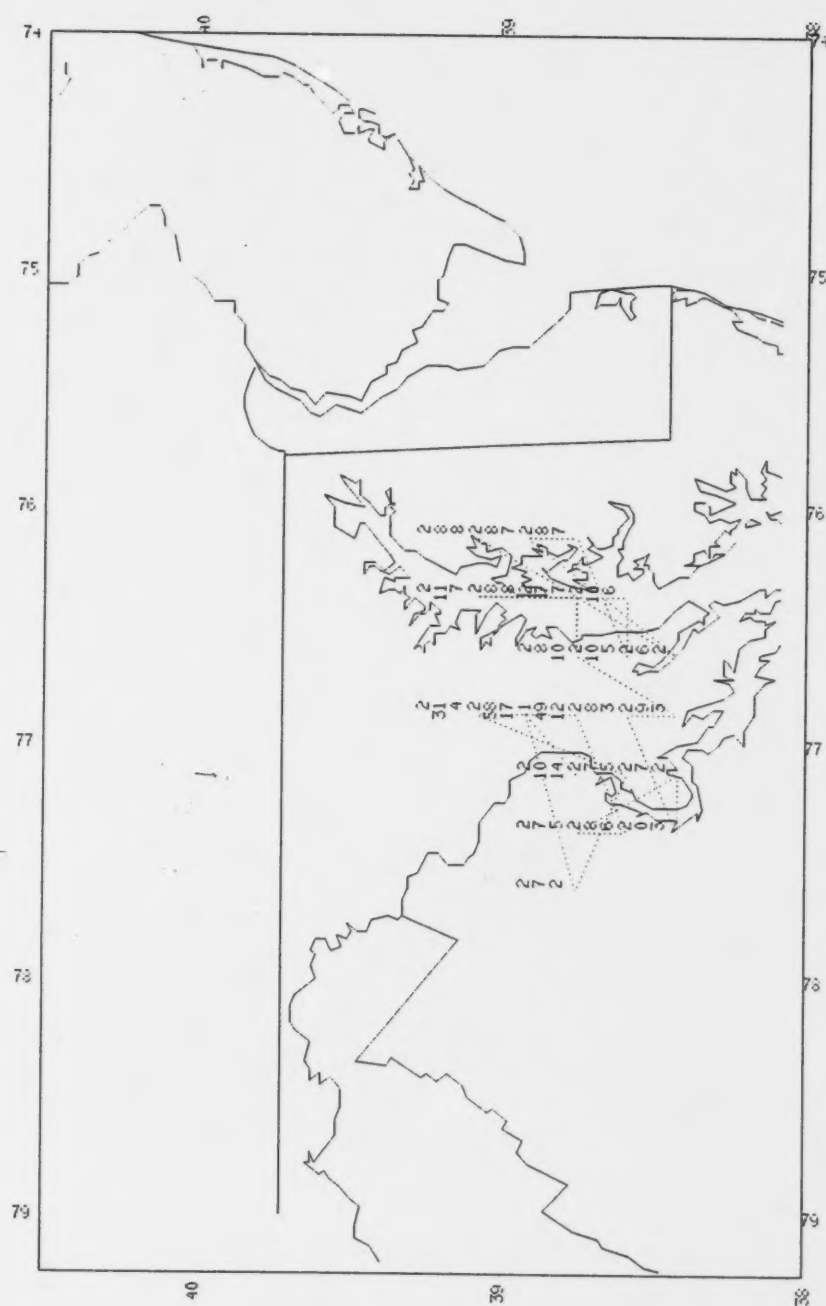


Figure 8.93. Geographical distribution of selected NO_x data from flight on July 25, 1980 in Washington, DC area. For each set of 3 numbers: top number is ROM layer, middle number is observed concentration (ppb), and bottom number is predicted concentration (ppb).



WASHINGTON, D.C. (EPA) 7/25/80 (HRS 9-15) NOx

WIDEVIEW extent - rows 1:15 cols 20:40

Figure 8.93 (cont.)

AIRCRAFT - WASHINGTON, D.C. AREA
JULY 25, 1980 (EPA)

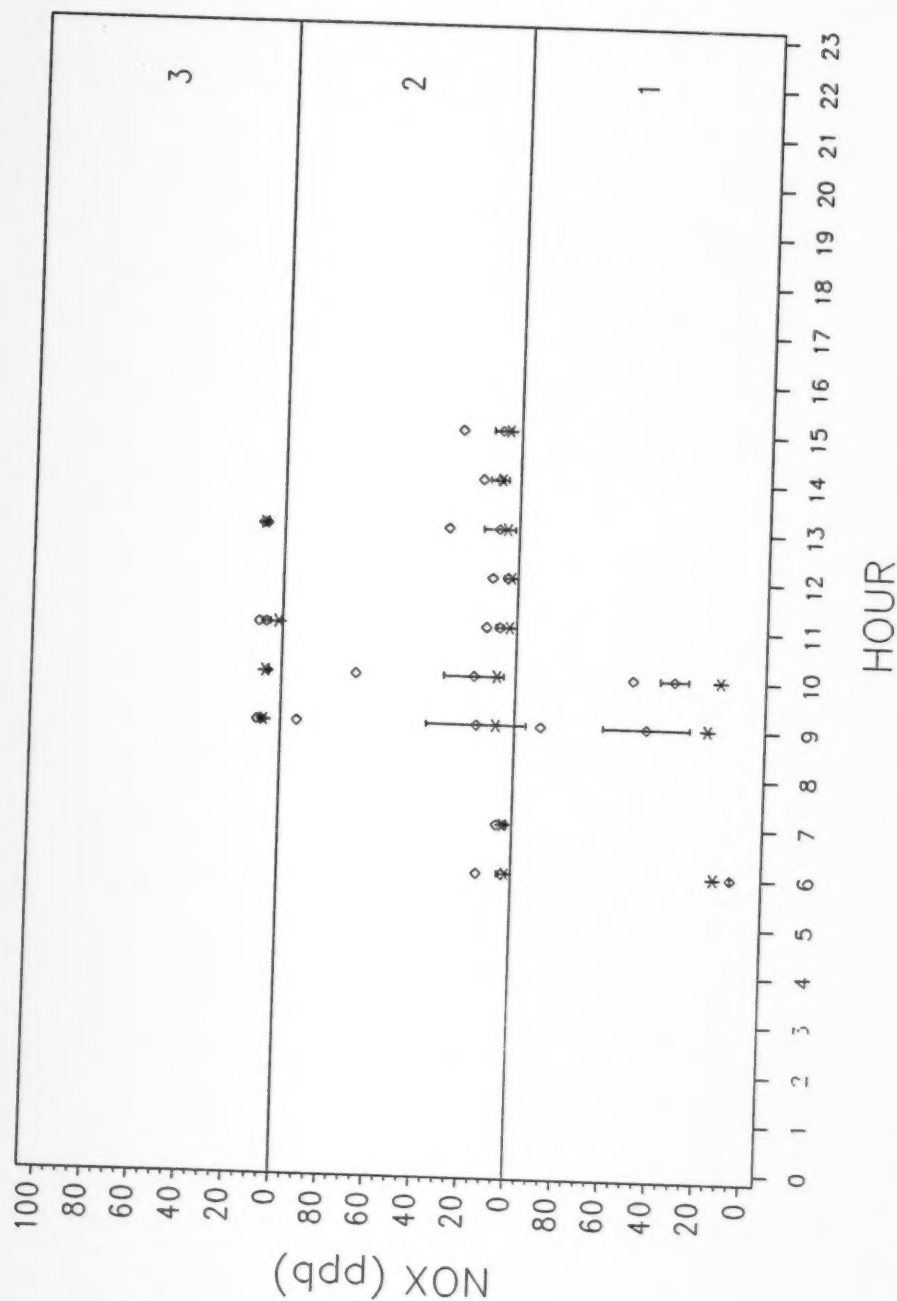


Figure 8.94. Time series of NO_x data from flight on July 25, 1980 in Washington, DC area. For each hour of the flight, all observed data within a given ROM layer are used to compute a mean concentration (diamond), surrounded by a standard deviation, and an observed maximum concentration (top diamond). The corresponding ROM prediction is indicated by an asterisk.

NMHC Aloft -- Baltimore, MD

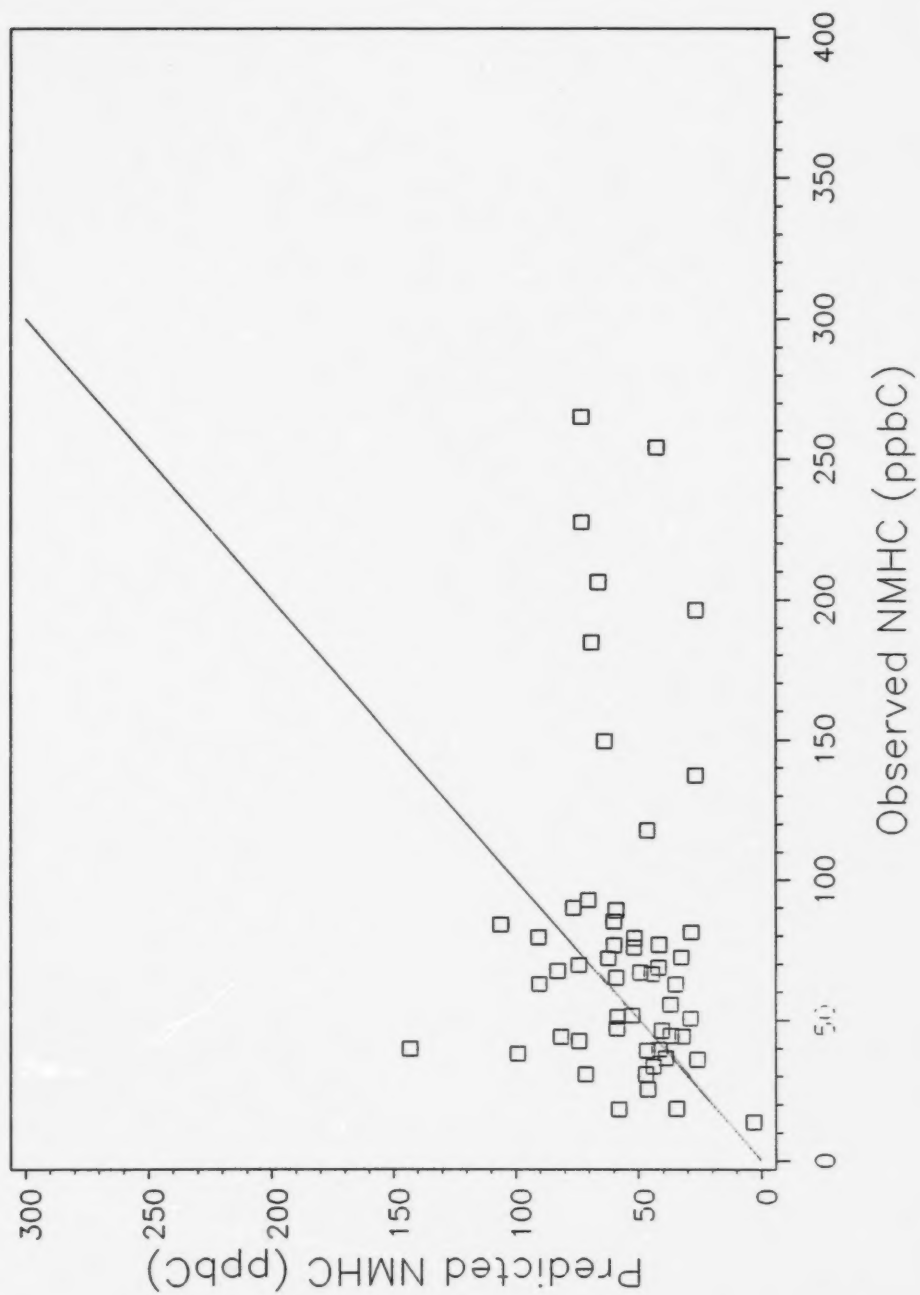


Figure 8.95. Scatterplots of observed (O) and predicted (P1) NMHC data aloft by urban area.

NMHC Aloft -- Boston, MA

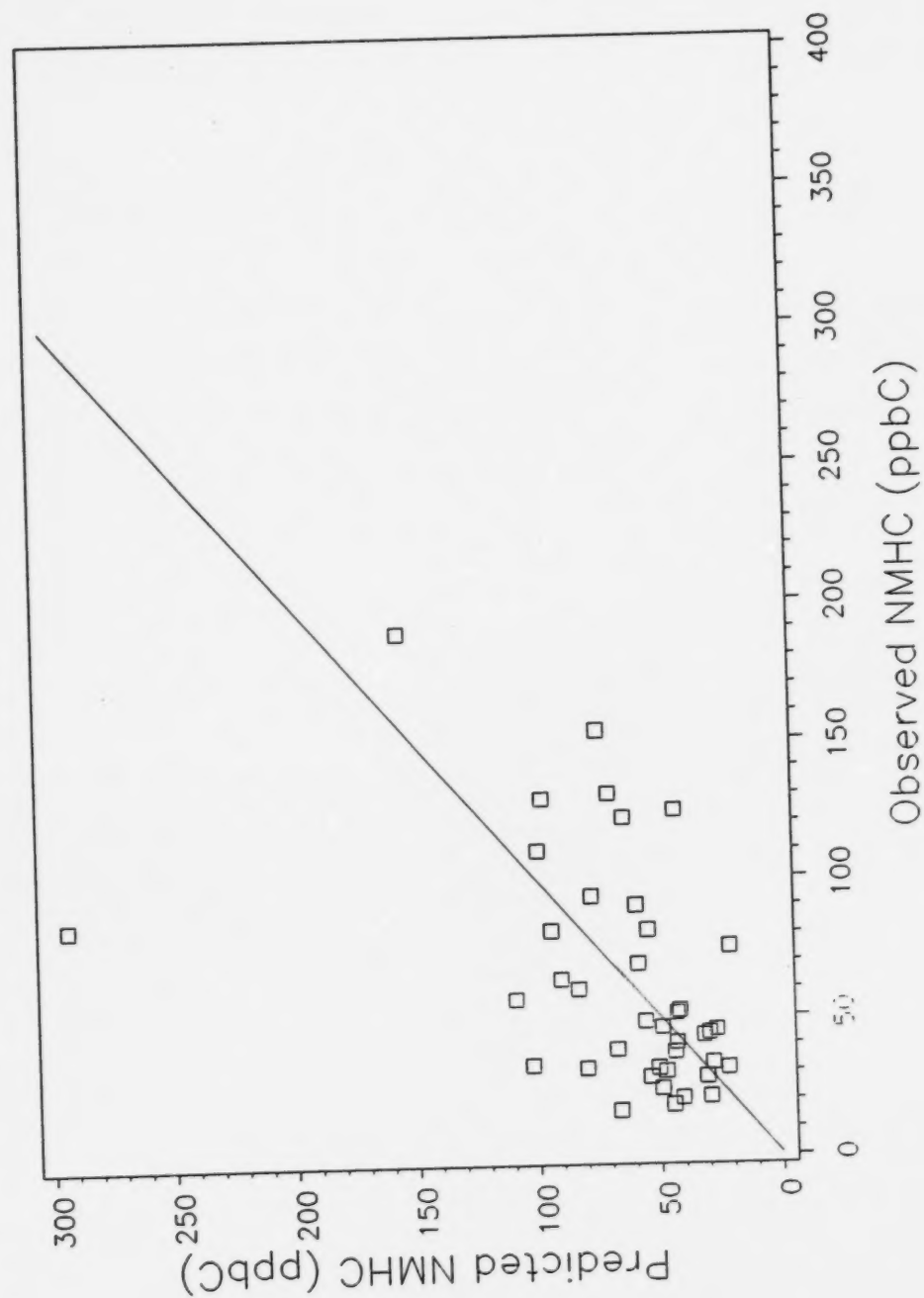


Figure 8.95 (cont.)

NMHC Aloft -- New York City

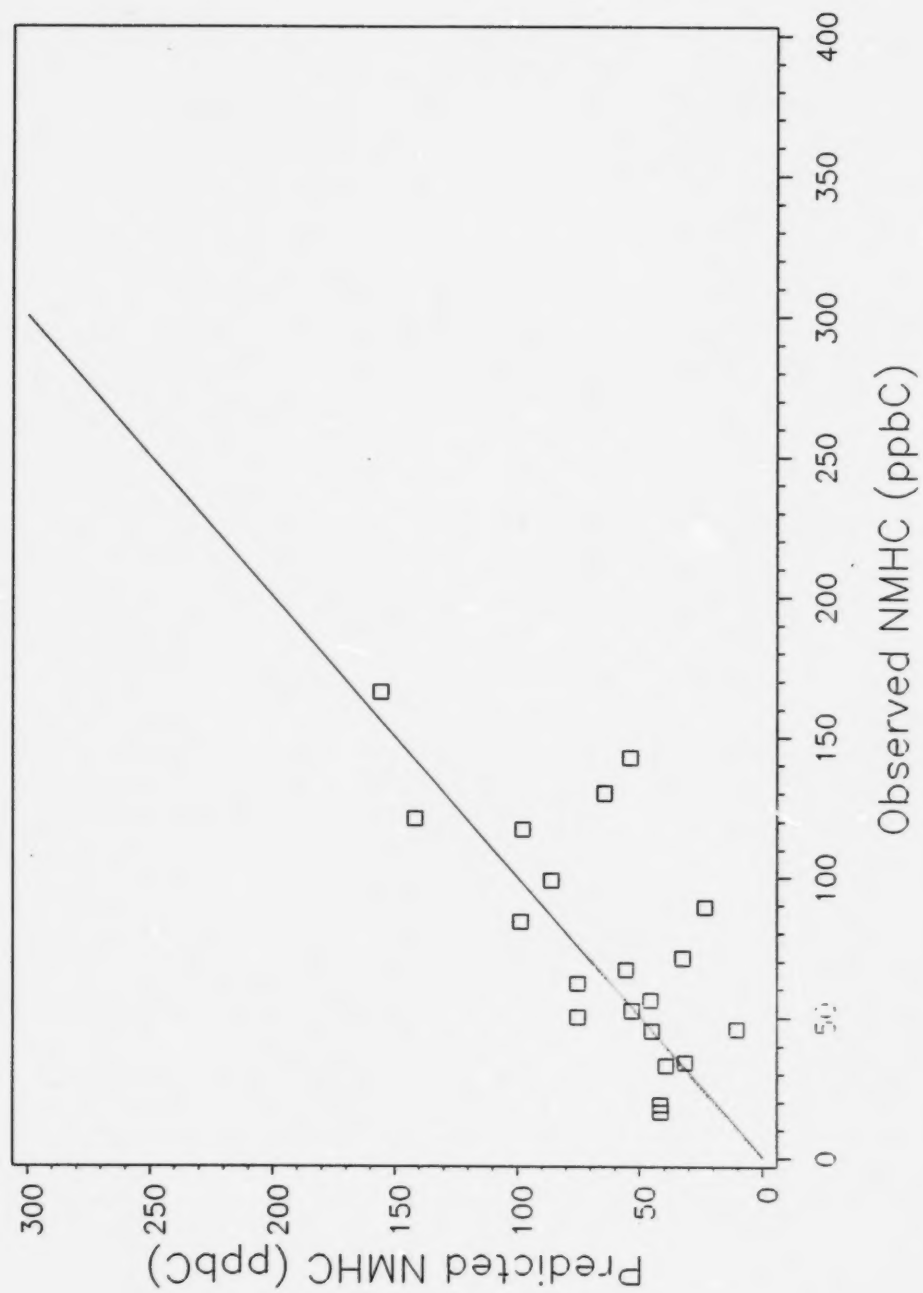


Figure 8.95 (cont.)

NMHC Aloft -- Washington, D.C.

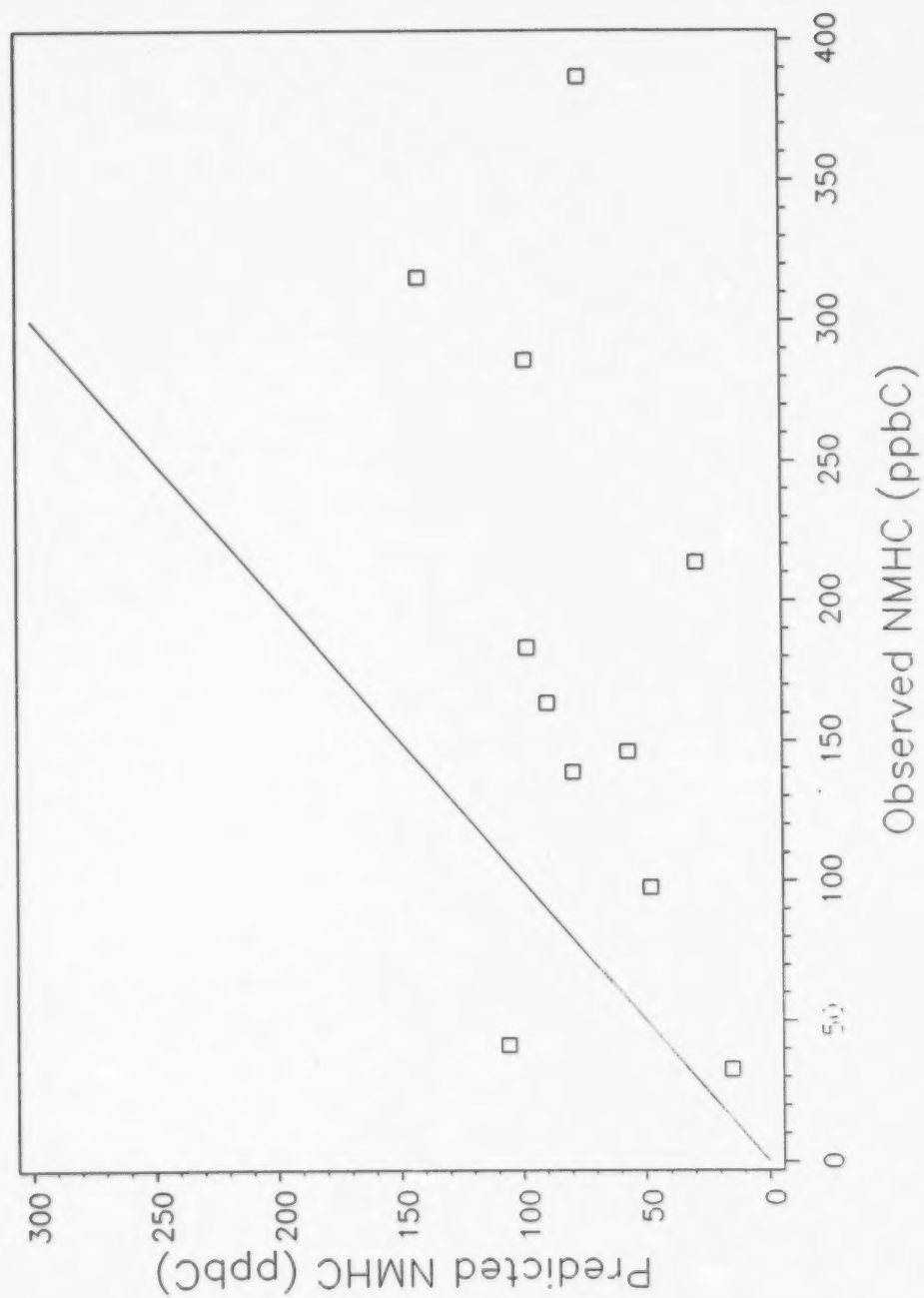


Figure 8.95 (cont.)

NMHC Aloft -- N.Y. - VT. Area

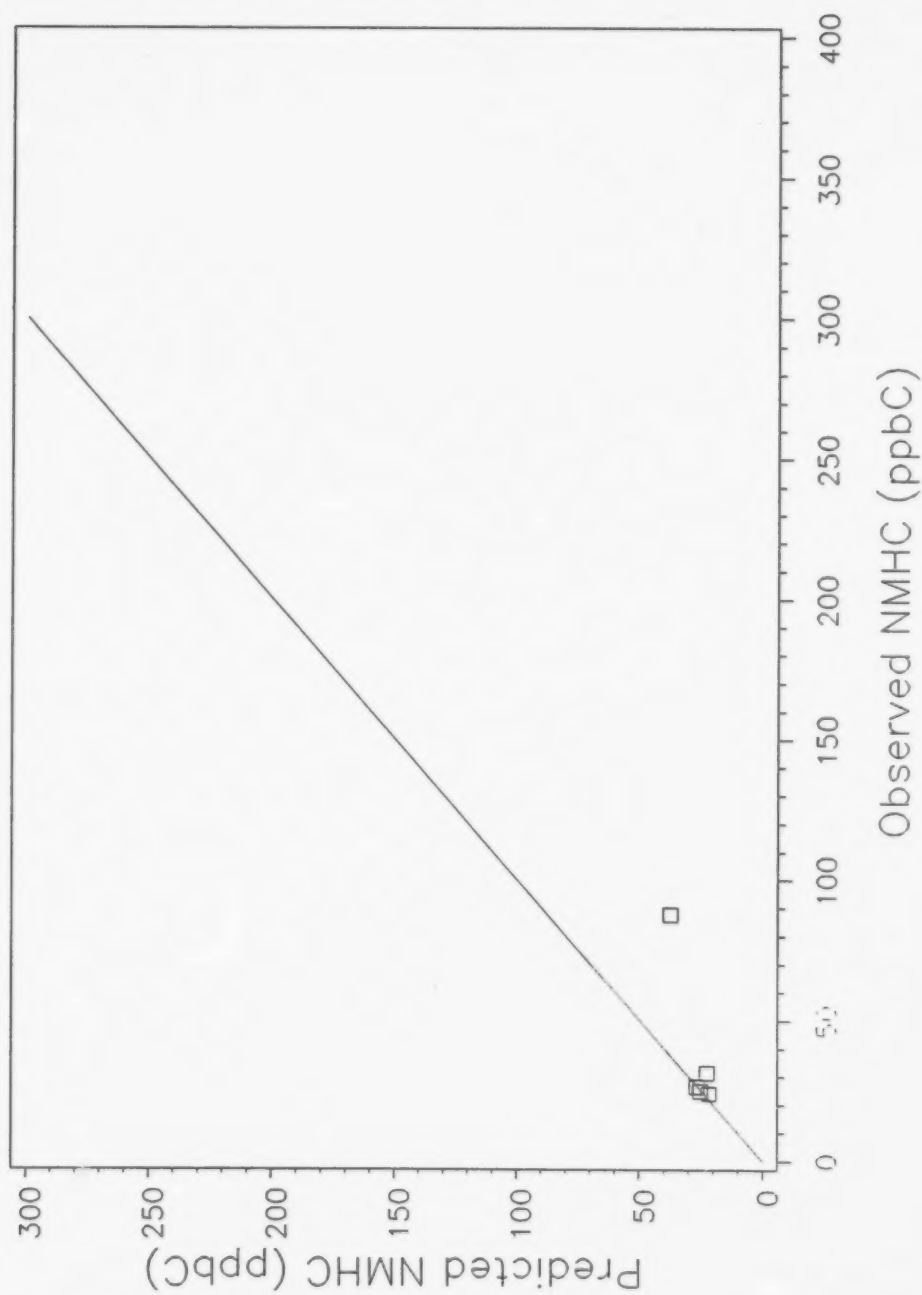


Figure 8.96. Scatterplots of observed (O) and predicted (P1) NMHC data aloft by non-urban area.

NMHC Aloft -- PA. -- MD. Area

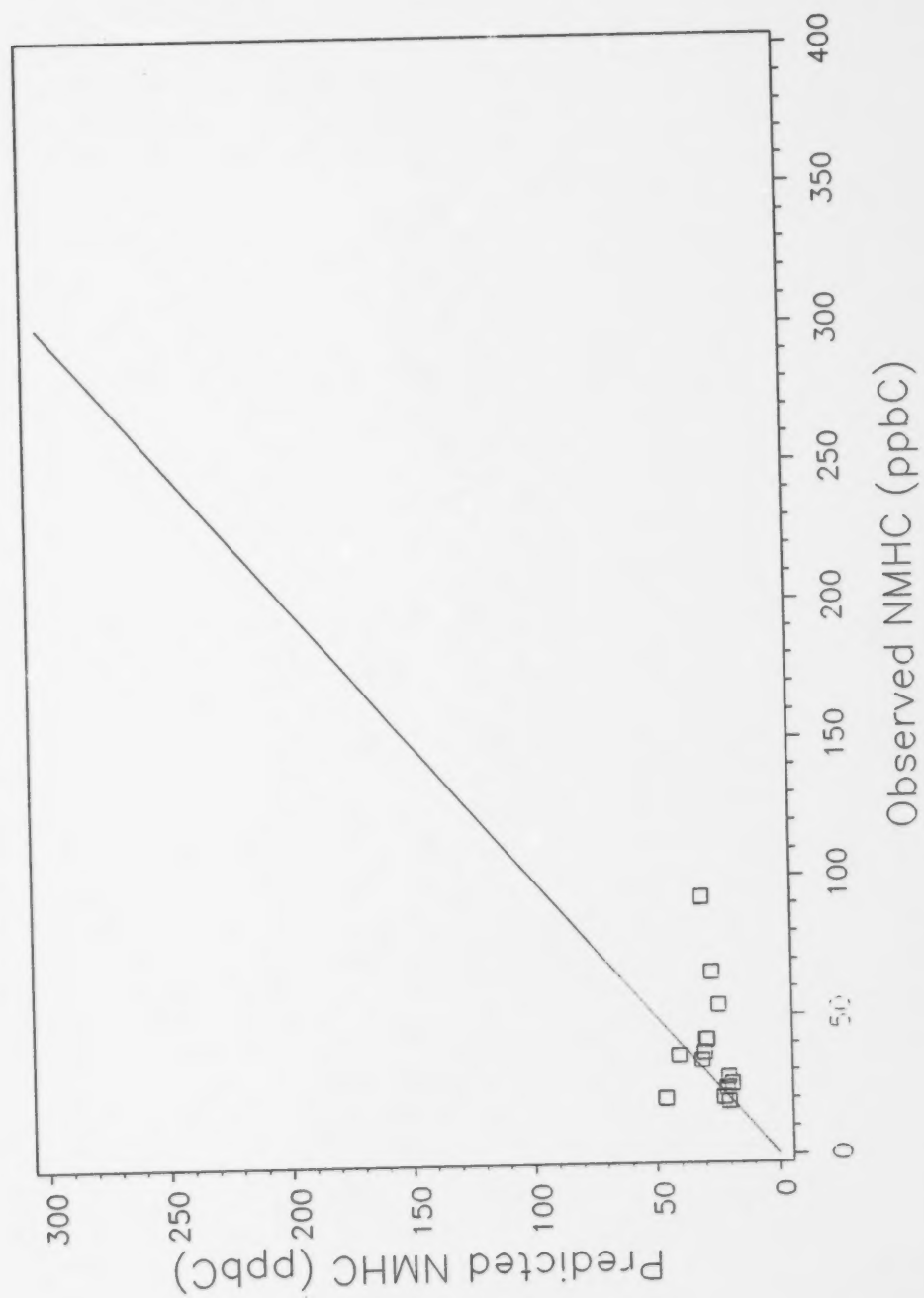


Figure 8.96 (cont.)

NMHC Aloft -- Ohio Area

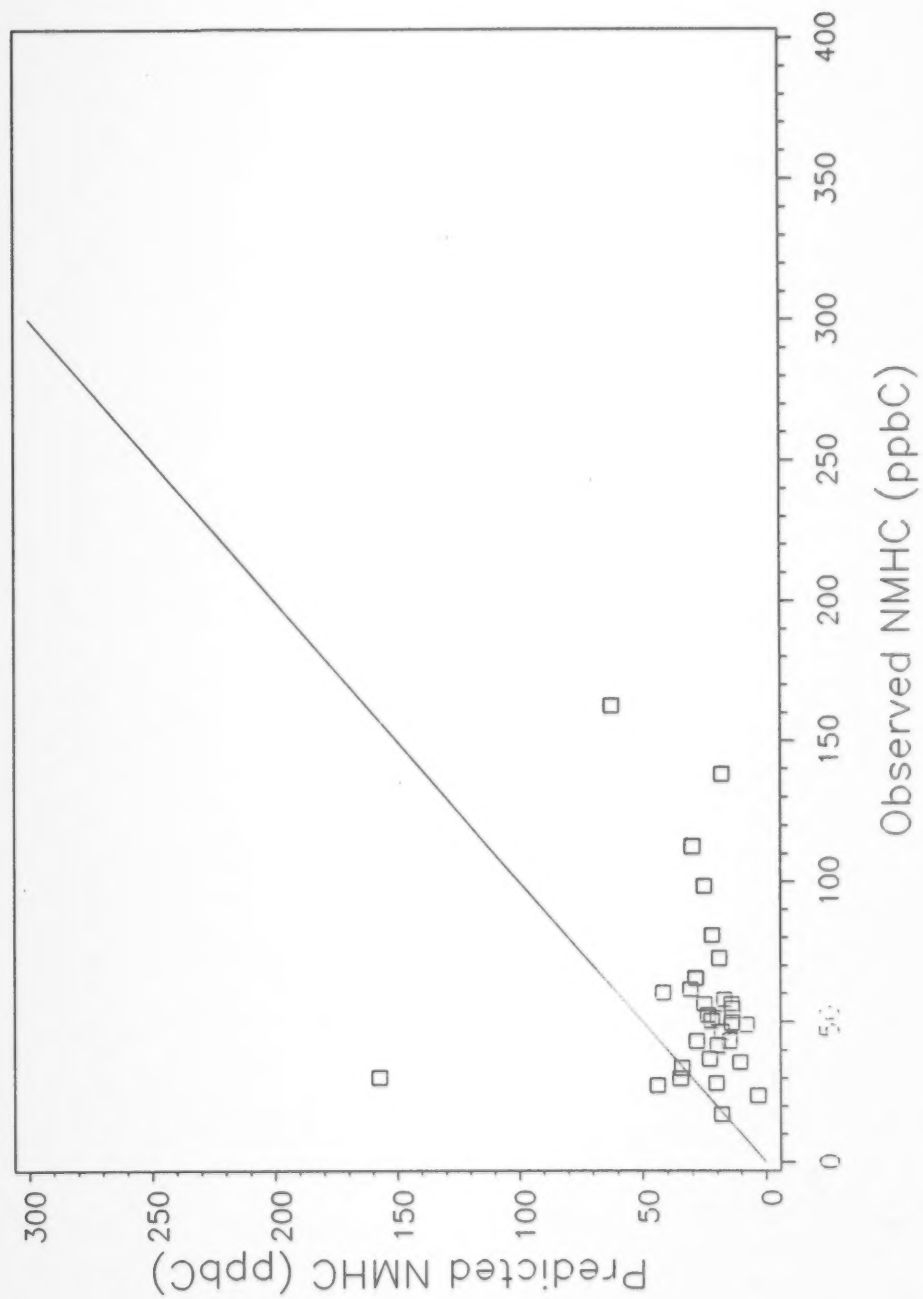


Figure 8.96 (cont.)

9 CONCLUSIONS AND RECOMMENDATIONS

EPA's second generation Regional Oxidant Model (ROM2.0) has been evaluated on the 1980 NEROS data base. This data base includes standard air quality data, including O_3 , NO_x , and NO_2 concentrations from the SAROAD and Canadian surface air quality monitoring data bases. It also includes special field study data on surface NMHCs and aircraft-measured O_3 , NO_x , NO_2 , and NMHCs in the Northeast U.S. Whenever possible, a quasi-deterministic approach to model evaluation was employed. This approach, as opposed to the fully deterministic approach, is thought to be more appropriate for models of regional and larger scales because of the problem of limited determinism in the regional wind fields. In the quasi-deterministic approach, data are aggregated both spatially and temporally to bring out the most meaningful elements of the model's performance. Where the quantity or quality of data did not permit a quasi-deterministic analysis, a more qualitative diagnostic analysis was performed.

The analysis using standard surface-monitored concentrations has shown that ROM2.0 predicts hourly O_3 concentrations above 80 ppb fairly well, and concentrations between 60 and 100 ppb particularly well. The average percentage of daylight hours (08–19 h, LST) over the simulation period showing concentrations above 80 ppb was 21.7% in the observed data set and 19.3% in the predicted data set for station groupings 1–3. These were the station groups which showed high to moderate values of observed O_3 concentrations. This statistic was compiled from data over the nearly 50 day simulation period spanning the summer of 1980. Cumulative concentration frequency distributions and histogram analyses of daytime hourly O_3 data have shown the model to typically predict a narrower overall concentration range than ambient observational data indicate. High hourly values are generally underpredicted and low values are overpredicted. This feature was evident in nearly all groups of monitoring stations. The cumulative frequency distributions treat the observed and predicted data sets independently for the simulation period. Thus, model behavior on individual days cannot be determined from this analysis. We use time series analyses for analysis of maximum O_3 concentrations to indicate behavior

within a group for individual days.

The model has shown good performance in predicting maximum daily O_3 concentrations averaged within station groups during the simulation period. The average daily maximum O_3 concentration over the simulation period for station group 1 was 88.1 ppb for the observed data set and 82.6 ppb for the predicted, a 6.2% underprediction. An examination of the time series of observed and predicted maximum O_3 concentrations, however, revealed that for this group there were often more significant differences between predictions and observations on any given day. At the 75th percentile level of daily maximum O_3 concentrations the ROM tended to underpredict by 30–50 ppb during episodic periods. For group 2, the average daily observed maximum was 76.9 ppb and the corresponding predicted value was 79.5 ppb, a 3.4% overprediction. For group 3, the observed maximum was 64.5 ppb and the predicted maximum was 70.1 ppb, a 8.7% overprediction. The time series analysis for group 3 showed that, on a daily basis, the median and 75th percentile levels of the maximum O_3 concentration showed better agreement between predictions and observations than did the group 1 results, with both over- and underpredictions occurring throughout the simulation period. The average performance over these three groups was a 2% overprediction of the daily maximum O_3 concentration.

A key indicator of model performance on the regional scale is the accuracy of simulating the spatial extent and location, as well as the magnitude of the pollutant concentrations within plumes from significant source areas on the regional scale, such as those emanating from major metropolitan areas within the model domain. ROM2.0 performance analyses in plume simulation were conducted for the Northeast Corridor sub-domain of NEROS, including the major metropolitan areas from New York through Boston. During episodic conditions during the simulation period, the urban plumes from Washington, Baltimore, New York and Boston could be clearly discerned in the model predictions. There was a systematic underprediction in the O_3 concentrations downwind of Philadelphia, often making it difficult to discern an integral urban plume. Because of the systematic nature of the phenomenon there is speculation that the NO_x emissions within the Philadelphia area may be overestimated. There is also evidence to this effect in the ROM2.0 performance analysis for NO_x concentrations.

The spatial pattern analysis has also indicated a significant bias in the wind field toward a westerly direction. For example, the wind transport in the model simulations often carries the New Jersey–New York metropolitan plume eastward over the ocean or over Long Island and Long Island sound. The plume, as judged from air quality data from the surface monitoring network however, is more often transported to the northeast over Connecticut and Rhode Island. The directional bias in transport is thought to derive from two sources, one correctable and the other more difficult to correct. An error in the ROM2.0 wind field processor (only recently

discovered) accounts for some of the bias, and the integration of the winds over relatively thick layers in the ROM accounts for the remainder. The latter problem is more difficult to correct conceptually because there is typically a natural turning of the winds from a westerly direction with increasing altitude, while the transport direction for plumes along the eastern seaboard is probably also greatly influenced by complex air-sea breeze regimes which are difficult to model on the regional scale. These regimes can cause significant departures from the mean flow captured in regional model wind fields. For those episodes in which the modeled winds agreed fairly well with the observed flow patterns, the New York, Washington-Baltimore, and Boston plumes were simulated quite well, especially in terms of plume location and spatial dimension. Maximum concentrations were usually underpredicted. The episodic maximum O_3 concentrations within the urban plumes was usually predicted between 180 and 200 ppb, while the maximum observed concentration range was 200–250 ppb.

An examination of the locations and number of surface monitoring stations for NO_x and NO_2 showed that there were problems with the regional representativeness of the surface-monitored concentrations. The mostly urban locations of these monitors meant that they were typically localized measurements. Aggregate groups of monitoring stations were formed for the major urban areas within the model domain. Results of model performance analyses for NO_x and NO_2 showed that the ROM2.0 significantly underpredicts NO_x and NO_2 among urban station groups at the 90th percentile of the cumulative concentration frequency distribution. At this percentile, the ratio of observed to predicted NO_x concentrations was 2.5 and the ratio for NO_2 was 1.9.

Spatial patterns of 06–09 h, LDT concentrations of NO_x and NO_2 were also analyzed for the Northeast Corridor sub-domain. Results of this analysis demonstrate that concentrations in this morning period also show factors of 2–3 model underprediction. Exceptions occur in the Toronto and Philadelphia areas where the model predictions of NO_x and NO_2 appear to be significantly higher than those in other areas. As mentioned above, this may infer overestimates of NO_x emissions for these areas. A confounding factor in the performance analysis for NO_x and NO_2 was the scarcity of significant areas of concentrations above 5 ppb, either in the model predictions or in the observations, for large areas of the domain. The accuracy of standard NO_x and NO_2 monitors degrades greatly below this level, and observed data cannot be trusted to be accurate when concentrations are less than 5 ppb.

Model performance on surface-derived NMHC concentrations was performed in a diagnostic manner because of the intermittancy of the measurements. All observed concentrations were calculated from a sum of the concentrations of individual species determined from gas chromatographic analyses of the NMHC samples. The ratios of observed to predicted NMHC concentrations averaged over the 06–09 h,

LDT period were generally in the range of 4–7 for large urban areas, and the ratio for afternoon hours *outside* of major urban areas was in the range of 1–3. Despite the large model underpredictions, an analysis of the carbon distribution among reactivity classes in the observed and predicted data sets showed quite good agreement in the relative distribution of carbon mass between higher and lesser reactive classes. The biogenic portion of the NMHCs (as judged by the explicitly modeled isoprene compound) did not show up consistently in the measured NMHC samples. It was therefore difficult to judge ROM2.0 performance on an absolute basis. The model predictions of isoprene concentrations, however, were in good agreement with surface values quoted in the literature from special field studies.

Model performance analyses using aircraft data were also performed in a diagnostic manner because of the intermittancy of the flights both in time and space. The analysis for O_3 concentrations shows that, in general, the overall background values in the planetary boundary layer do not build up as high under episodic conditions in the predictions as they do in the observations. Typically, regionwide O_3 concentrations predicted by ROM2.0 were in the 40–60 ppb range, while corresponding concentrations measured by aircraft monitors were 40–90 ppb, with the higher observed values occurring under strong episodic conditions. Most instances of regionally elevated O_3 values were underestimated by 20–30 ppb. Ozone aloft in the morning, upwind of urban areas, was generally underpredicted on days when aircraft measurements showed values greater than ≈ 70 ppb. The regional background O_3 underprediction by the ROM was, however, not a totally pervasive phenomenon. Examination of predicted spatial patterns reveals the model to predict large areas of >80 ppb concentrations which build up, especially during daytime hours, and are transported through the model domain. These areas often merge with each other as they grow larger and are moved by the transport fields. Typically, they shrink in size after the sun sets and gradually dissipate over the nighttime hours. Ambient patterns, as judged by the intermittent aircraft observations, appear to show more widespread areas of >80 ppb O_3 concentrations under episodic conditions. These areas also apparently do not shrink in size and magnitude over the nighttime period as much as the ROM predictions suggest, as judged by the early morning aircraft flights. Background values of NO_x were also underpredicted, by factors of 2–3. Observed values of NO_x concentration were often in the 5–10 ppb range on regional flights with predictions along the same flight path typically less than 5 ppb.

Flights conducted in and downwind of urban areas showed ROM's O_3 concentration predictions to be very credible, especially when model wind fields provided transport along the Northeast Corridor from a southwesterly direction. The urban plumes simulated downwind of Boston, New York, and Washington especially showed good agreement with aircraft observations. The ROM tended to underpredict the maximum concentration areas within the plumes, although the degree of underprediction was not great for concentrations as high as 150–180 ppb. For ob-

served concentrations over 200 ppb, as measured by aircraft monitors, the model underprediction was generally more substantial. Model performance for NO_x concentrations observed in the aircraft data shows ROM2.0 to generally underpredict, with observed to predicted ratios of $+5$ ppb NO_x in the range of 1–2. These ratios were generally somewhat less than those for the corresponding NO_x ratios in the aircraft background measurements and for the surface concentration analyses. Concentrations of NMHC aloft during the morning period were observed to be considerably lower (by up to a factor of 10 or more) than the morning surface NMHC concentrations. ROM2.0 still generally underpredicted the NMHC concentrations observed from aircraft samples, but by a smaller factor (1–3, as opposed to 4–7 in the surface data).

Overall, the techniques used in this performance evaluation proved to be instructive for eliciting overall regional model performance. Spatial pattern analyses and cumulative concentration frequency distributions were especially helpful in this regard. We have avoided strict pairing of observed and predicted concentrations for this regional model evaluation because of the strong possibility of misleading interpretations from such analyses on the regional scale. This deterministic method is more appropriate for smaller scale models used on fairly dense monitoring networks. The eventual move to a fully probabilistic method of regional model application and performance evaluation is still our goal.

It is clear from our study that a critical factor in the utility of regional model results is the correct simulation of the location of regional concentration patterns, especially from urban area plumes. The important factor in the vicinity of major urban areas is the correct simulation of the mixing of upwind, over, and downwind air concentrations. Providing accurate wind fields to regional models will help insure this. We are attempting to correct some of the transport biases discovered in ROM2.0 from this performance evaluation. The problem of localized circulation features that often exist on scales smaller than the existing meteorological monitoring network will still remain. For Northeast Corridor cities, these local circulations may greatly influence plume transport patterns. Ultimately, a nested scale predictive meteorological model may be needed to generate the transport fields used in ROM to most accurately model plume transport on regional scales in areas of complex flow.

While the overall performance of ROM2.0 for predicting O_3 concentrations has not shown sufficient cause for rejecting use of the model in regulatory analyses,¹ a number of issues have arisen that prevent recommending use of the model in a simple, unassisted manner for studies involving violations of the O_3 air quality standard. These include the day-to-day variability of model bias results, the systematic

¹Model evaluation studies, such as this one, will not indicate model acceptance, but rather will only indicate whether model rejection is warranted. Model acceptance comes only after non-rejection in many evaluation studies over time.

transport biases seen in the spatial patterns, and perhaps most importantly, the general underprediction of regional background O_3 concentrations under episodic conditions. For applications studies, such as the upcoming ROMNET (Regional Oxidant Modeling for Northeast Transport) project, the ROM results must be used with care. Episodes must be chosen for which the model is operating at its most consistent level with best fidelity. Careful analysis of the simulated transport patterns and background O_3 levels must be made for a given episode before model results can be used for subsequent analysis. Sensible guidance for use of ROM results will require strong interaction of the modelers, with their insights and ability to interpret model results, and the regulatory users of the information.

This model performance study has also raised some key questions concerning the data base with perhaps the greatest inherent uncertainty, the emissions inventory. The large and consistent underprediction of NMHCs seems to indicate deficiencies in the hydrocarbon portion of the inventory. These deficiencies may be across the board on all sources since the normalized carbon fractions seem to agree fairly well in the observations and predictions of NMHC reactive classes. Inconsistencies in the NO_x results, such as the relatively high values for Toronto and Philadelphia NO_x predictions compared to even larger cities, may imply that inventory techniques are not consistent from state to state or country to country (at least in the case of the U.S. and Canada). Missing or incorrect temperature sensitivities of both biogenic and anthropogenic precursor emissions may be responsible, in part, for the failure of the model to build the background tropospheric O_3 concentration levels as high as they have been observed from field study results during episodic conditions. Current efforts toward the development of a 1985 base year emissions inventory by NAPAP will take steps to rectify some of the known deficiencies in the 1980 inventory. Several previously uninventoried NMHC source categories will be included in the 1985 inventory, including the potentially major category of mobile source evaporative running losses. In addition, day-specific temperature corrections of evaporative NMHC emissions from mobile and other sources in the Northeast U.S. will be made to the 1985 inventory for subsequent use in future ROM modeling.

The remaining emission inventory questions must be resolved if we are to ever evaluate the performance of air quality models in the capacity of their most common use for air quality planning. That is, we must evaluate $\partial O_3 / \partial S$, where S is emissions for various base and post-control emission inventories. Because of monitoring deficiencies, different methodologies used in successive versions of emissions inventories separated over time, and large inherent uncertainties in the emissions estimates we are a long way from this type of model evaluation. This must, however, be a long range goal.

Finally, to complete the picture of model performance evaluation, there must be a corresponding model sensitivity study. A systematic sensitivity study of a complex regional model such as ROM is a very resource-intensive task, and was

outside the scope of the present effort. Results from a sensitivity study will, among other purposes, help guide the application of resources to narrow the uncertainty in those required data for which the model is most sensitive. Results from a model evaluation study, such as this one, will help to provide invaluable guidance toward establishing some of the critical sensitivity tests. We hope to begin such a sensitivity study soon. The combination of performance evaluation and sensitivity results is key to understanding *why* a model has performed in the manner it has under varying conditions.

Model performance is a continuing task. Once a model is used in production for multiple applications some type of performance study is required for each application. Even though the science embodied in the model may be up to contemporary standards, the stochastic nature of the atmosphere can cause variations in model performance from location to location and from time to time. Detailed data bases, including aircraft based measurements, such as those used in this study, are not commonly available. However, the methods of evaluation demonstrated here may also be applied to routinely available data bases for less rigorous evaluation exercises.

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